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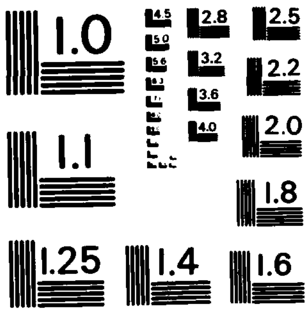

MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

1982

AFOSR/AFRPL

ROCKET PROPULSION

RESEARCH MEETING

2-4 MARCH 1982

ESSEX HOUSE

LANCASTER, CALIFORNIA

ADA 116-080

AFOSR/AFRPL ROCKET PROPULSION RESEARCH MEETING

Leonard H. Caveny, et al

Essex House
Lancaster, CA

1982

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REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: AFOSR-TR- 82-0507	2. GOVT ACCESSION NO.: AD-A1[illegible]
3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle): AFOSR/AFRPL ROCKET PROPULSION RESEARCH MEETING - 1982 -	5. TYPE OF REPORT & PERIOD COVERED: INTERIM MARCH 1981 - FEBRUARY 1982
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s)/Editor(s): LEONARD H CAVENY, DAVID M MANN	8. CONTRACT OR GRANT NUMBER(s): In-House
9. PERFORMING ORGANIZATION NAME AND ADDRESS: AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NA, BOLLING AFB, DC 20332	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: 61102F 2308/A1, A3, M1 2307/M1, 2303/M1
11. CONTROLLING OFFICE NAME AND ADDRESS: Same	12. REPORT DATE: FEBRUARY 1982
	13. NUMBER OF PAGES: 128
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report): UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

*Air Force Rocket Propulsion Laboratory
Edwards AFB, CA 93534

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

ROCKETS, COMBUSTION, ENERGETIC MATERIALS, PROPELLANTS, CHEMICAL KINETICS, THERMAL PROPERTIES, THERMAL PROTECTION, EXHAUST PLUMES, COMBUSTION STABILITY, ACOUSTICS, STRUCTURAL MECHANICS

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This document contains expanded abstracts from the 1982 meeting on the Air Force basic research program on energy conversion relating to rocket propulsion. The meeting (Lancaster, CA on 2-4 March 1982) presented research supported by both the Air Force Office of Scientific Research and the Air Force Rocket Propulsion Laboratory. Major topics included: diagnostics of reacting flows, combustion, chemical kinetics, thermal properties, propulsion concepts, energetic materials, material and propellant ingredients, exhaust plumes, transition to detonation, combustion stability, structural mechanics.

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Agenda Summary

Agenda of Individual Presentations

Abstracts — See p. A-10

Appendix 1 - Diagnostics in Reacting Media

Appendix 2 - Overview of Rocket Propulsion Research Goals

Appendix 3 - Space Power and Propulsion (FY83 Initiative)

Table of Contents of Abstracts — p. A-10

PREFACE

The meeting includes presentations from both the AFOSR and AFRPL basic research programs. Thus, during the three days, the attendees will be able to gather a reasonably complete picture of the Air Force research program on rocket propulsion and reacting flows. The meeting on Advanced Diagnostics of Reacting Flows was held at Stanford University on 25-26 February 1982; the book of abstracts for that meeting is available from AFOSR.

We are using a very specific format for the abstracts. The body of each abstract begins with a short statement of relevant scientific questions addressed by the research, followed by an explanation of the approach. A statement of the uniqueness of each approach was solicted. The major portion of the text is devoted to a discussion of results obtained since last years meeting. The abstracts describe two figures: Figure 1 illustrates the main features of the approach and Figure 2 presents a primary accomplishment.

Hard copies of the vugraph material and backup information are in file folders (one for each presentation) which are placed on a table at the rear of the meeting room. Thus, it can be referred to by anyone in the audience either before or after the presentations.

One of the primary objectives of this meeting is to encourage the attendees to consider new research approaches. Since a 25 to 30 percent annual turn-over is built into program, each year there are ample opportunities for new research approaches and for new principal investigators. The list of presentations indicates the research efforts which have begun since July 1981. Several of the presentations are intended to give guidance on research directions for the next five to ten years. Encouragement is given to bold approaches to the most challenging goals. However, responses of prospective principal investigators should not be limited by the stated goals. The location of this meeting promotes interchanges among the attendees by being held near organizations interested in this research. Of course, the attendees are encouraged to establish communications with their technical counterparts within the Air Force. Also, questions can be directed to either,

Leonard H Caveny	or	David M Mann
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Bolling AFB		Edwards AFB, CA 93534
Washington, DC 20332		
(202) 767-4937 or AV297-4937		(805) 277-5206 or AV350-5206

Appendices have been included in to provide additional information on research opportunities.

AGENDA SUMMARY

1982 AFOSR/AFRPL ROCKET PROPULSION RESEARCH MEETING

ESSEX HOUSE
Lancaster, CA

2-4 March 1982

LIST OF SESSIONS

March 2 - Tuesday

0800	Registration (Lancaster Room 1)
0830	Announcements
0835	WELCOME by Don A Hart, Director, AFRPL
0845-1100	Unsteady and Reacting Flows
1100-1130	AFOSR Interests in Rocket Propulsion, Leonard H Caveny, AFOSR
1300-1530	Propulsion
1530-1645	Structural Mechanics
1645-1715	Administrative Meeting for AFOSR Contractors

March 3 - Wednesday

0745	Late Registration (Lancaster Room 1)
0800-1200	Combustion
1300	Air Force Propulsion Requirements in 1990 to 2000 Richard R Weiss, Chief Scientist, AFRPL
1330	AFRPL Research Interests in Rocket Propulsion, David M Mann, AFRPL
1400-1700	Thermodynamics and Kinetics
1730-1900	Social Hour (Cash Bar) - Nina's Supper Club (Essex House)

March 4 - Thursday

0745	Late Registration (Lancaster Room 1)
0800-1200	Advanced Energetic Ingredients
1300-1530	Rocket Exhaust Plumes
1530-1730	Metalized Propellants
1730	Adjourn Meeting

(21 Dec 1981/LHC 0053G)

1982 AFOSR/AFRPL ROCKET PROPULSION RESEARCH MEETING

ESSEX HOUSE
Lancaster, CA

Tuesday AM
2 March 1982

TIME NUM.
0800 REGISTRATION - (Lancaster Room 1)

Session Chairman: Leonard H Caveny, AFOSR/NA

0830 ANNOUNCEMENTS

0835 WELCOME: Don A Hart, Director, AFRPL

Topic: Unsteady and Reacting Flows

0845 1 ROCKET MOTOR AEROACOUSTICS. Warren C Strahle, Georgia Institute of Technology, Atlanta, GA

0915 2 COUPLING BETWEEN VELOCITY OSCILLATIONS AND SOLID PROPELLANT COMBUSTION. Robert S Brown, Paul G Willoughby, and R C Waugh, Chemical Systems Division of United Technologies Corp, Sunnyvale, CA

0945 3 INTERNAL FLOW FIELDS AND VELOCITY COUPLING. Moshe BenReuven and Martin Summerfield, Princeton Combustion Research Laboratories, Inc, Princeton, NJ

1015 Break

4 *INVESTIGATION OF VELOCITY AND PRESSURE COUPLED ADMITTANCES OF ALUMINIZED AND NONALUMINIZED PROPELLANTS. Ben T Zinn and Brady R Daniel, Georgia Institute of Technology, Atlanta, GA

1030 5 NONLINEAR COMBUSTION MODELING. Joseph Baum, University of Dayton Research Institute, Dayton, OH and J Levine, AFRPL/PAC

1100 6 OVERVIEW: AFOSR INTERESTS IN ROCKET PROPULSION. Leonard H Caveny, AFOSR/NA

1130 LUNCH (Reconvene at 1300)

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*Will be presented at 1130 3 March.

Tuesday PM
2 March 1982

Session Chairman: Robert Vondra, AFRPL/LKDH

Topic: Propulsion

TIME	NUM.	
1300	7	SOLID PROPELLANT AIRBREATHING COMBUSTION RESEARCH. Warren C Strahle, James E Hubbartt and J I Jagoda, Georgia Institute of Technology, Atlanta, GA
	8	*FUEL-RICH SOLID PROPELLANT BORON COMBUSTION. Merril King, Ronald S Fry, and James Komar, Atlantic Research Corp, Alexandria, VA
1330	9	CAPILLARY DISCHARGE IONIZATION. Julius Perel and John F Mahoney, Phrasor Scientific, Inc, Duarte, CA
1400	10	THE POTENTIAL FOR USING ELECTROMAGNETIC ENERGY TO SUPPLY PROPULSION ENERGY. Charles L Merkle, Pennsylvania State University, University Park, PA
1430	11	ELECTROMAGNETIC ACCELERATION OF ROTATING CHARGES. Michael M Micci, Pennsylvania State University, University Park, PA (new start)
1445		Break
1500	12	SOLID ROCKET AND SPACE PROPULSION STUDIES. Robert L Glick, Purdue University, West Lafyette, IN (new start)

Topic: Structural Mechanics

1515	13	STRUCTURAL MECHANICS RESEARCH. C T (Jimmie) Liu, AFRPL/MKPB (New Start)
1545	14	PROPELLANT NONLINEAR CONSTITUTIVE THEORY EXTENSION. Gene Francis, Chemical Systems Division, United Technologies, Sunnyvale, CA
1615	15	THERMOMECHANICALLY COUPLED VIBRATIONS IN A CYLINDRICAL GEOMETRY LACKING SYMMETRY; A FINITE ELEMENT SOLUTION PROCEDURE. Richard W Young, University of Cincinnati, Cincinnati, OH
1645		ADJOURN SESSION
1645		ADMINISTRATIVE MEETING FOR AFOSR CONTRACTORS ONLY

AIAA LOCAL SECTION MEETING

1830	Mixer
1900	Dinner
2000	Program (to be announced)

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*Presentation will not be made but vugraph material is available at rear of meeting room.

Wednesday PM
3 March 1982

Session Chairman: Lawrence P Quinn, AFRPL/MKBN

TIME	NUM.	
1300	22	AN OVERVIEW: AIR FORCE PROPULSION REQUIREMENTS IN 1990 TO 2000. Richard R Weiss, Chief Scientist, AFRPL
1330	23	AFRPL RESEARCH INTERESTS IN ROCKET PROPULSION. David M Mann AFRPL/XRX

Topic: Thermodynamics and Kinetics

1400	24	EVALUATION AND COMPILATION OF THE THERMODYNAMIC PROPERTIES OF HIGH TEMPERATURE SPECIES. Malcom W Chase, The Dow Chemical Company, Midland, MI
1430	25	CRITICAL EVALUATION OF HIGH TEMPERATURE CHEMICAL KINETIC DATA. Norman Cohen, K Westberg, Aerospace Corporation, Los Angeles, CA and Lewis Gevantman, National Bureau of Standards, Gaithersburg, MD
1500		Break
1530	26	CARBON-CARBON PROCESSING VARIABLES INVESTIGATION. Wesley P Hoffman, AFRPL/MKBN
1600	27	METAL COMBUSTION KINETICS. James F Driscoll and J Arthur Nicholls, University of Michigan, Ann Arbor, MI
1630	28	THERMOPHYSICAL PROPERTY DETERMINATIONS USING TRANSIENT TECHNIQUES. Raymond E Taylor, R L Shoemaker and Leslie Koshigoe, Purdue Univ, West Lafayette, IN (New Start)
1730		SOCIAL HOUR (Cash Bar), Nina's Supper Club

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*Presentation will not be made but vugraph material is available at rear of meeting room.

Wednesday AM
3 March 1982

0745 Late Registration (Lancaster Room 1)

Session Chairman: Wayne E Roe, AFRPL/PAC

Topic: Combustion

TIME	NUM.	
0800	16	COMBUSTION MODELING OF SOLID PROPELLANTS. Merrill W Beckstead, Brad Eldridge, and Richard Raun, Brigham Young University, Provo UT
0830	17	COMBUSTION MECHANISMS. David P Weaver, AFRPL/PAP
0900	18	COMBUSTION MECHANISMS. David Campbell, University of Dayton Research Institute.
0930	19	MODELING OF DEFLAGRATION TO SHOCK TO DETONATION TRANSITION (DSDT) IN GRANULAR SOLID PROPELLANTS. Herman Krier, University of Illinois at Urbana-Champaign, Champaign, IL
1000		Break
1030	20	NON-STEADY COMBUSTION OF COMPOSITE PROPELLANTS. Leon D Strand and Norman S Cohen, Jet Propulsion Laboratory, Pasadena, CA
1100	21	NITRAMINE COMBUSTION MODELING. Moshe BenReuven, Princeton Combustion Research Laboratory, Inc, Princeton, NJ
1130	4	INVESTIGATION OF VELOCITY AND PRESSURE COUPLED ADMITTANCES OF ALUMINIZED AND NONALUMINIZED PROPELLANTS. Ben T Zinn and Brady R Daniel, Georgia Institute of Technology, Atlanta, GA
1200		LUNCH (Reconvene at 1300)

Thursday AM
4 March 1982

0745 Late Registration (Lancaster Room 1)

Session Chairman: Frank Roberto, AFRPL/MK

Topic: Advanced Energetic Ingredients

TIME	NUM.	
0800	29	HIGH ENERGY PROPELLANT MARERIALS RESEARCH: A TECHNICAL ASSESSMENT. Donald L Ross, Marion E Hill, Clifford D Bedford, and Robert W Woolfolk, SRI-International, Menlo Park, CA 94025
0830	30	NEW SYNTHETIC TECHNIQUES FOR ADVANCED PROPELLANT INGREDIENTS: SELECTIVE CHEMICAL TRANSFORMATIONS AND NEW STRUCTURES. Scott A Shackelford, AFRPL/LKLR (New Start)
0900	31	MECHANISTIC STUDIES OF NITRAMINE AND ADVANCED PROPELLANT INGREDIENT INITIAL THERMOCHEMICAL DECOMPOSITION: 2303 MI SN. Berge B Goshgarian, AFRPL/LKLR
0930	32	I. SYNTHESIS OF HYDROXY-TERMINATED DINITROPROPYL ACRYLATE POLYMERS. II. IMPROVED CHARACTERIZATION OF HYDROXY-TERMINATED PREPOLYMERS. C Sue Kim, California State University at Sacramento, Sacramento, CA
1000		Break
1030	33	STRUCTURE-PROPERTY RELATIONSHIPS IN POLYETHER ELASTIMERS. Stan Morse, University of Dayton Research Institute, Dayton, OH
1100	34	KINETICS AND THERMODYAMICS OF THE BETA TO DELTA HMX TRANSFORMATION: AN APPROACH TO ALTERING THE NATURE OF HMX. Thomas B Brill, Richard J Karpowicz, and Thomas M Haller, University of Delaware, Newark, DE
1130	35	HMX COMBUSTION MODIFICATIONS. Joseph E Flanagan, Milton B Frankel, Rocketdyne Division, Rockwell International, Canoga Park, CA
1200		LUNCH (Reconvene 1300)

Thursday PM
4 March 1982

Session Chairman: Wilbur C Andrepont, AFRPL/DYP

Topic: Rocket Exhaust Plumes

TIME	NUM	
1300	36	VAPOR PRESSURE OF SALT-HCl-H_2O SOLUTIONS BELOW 0 C. Eugene Miller, University of Nevada, Reno, NV
1330	37	FLOW OF GAS-PARTICLE MIXTURES. Melvyn C Branch, University of Colorado, Boulder, CO
1400	38	ADVANCE COMBUSTION/PLUME DIAGNOSTICS. Jay D Eversole, University of Dayton Research Institute, Dayton, OH
1430	39	COMBUSTION KINETICS OF METAL OXIDES AND HALIDE RADICALS AND METAL ATOMS. Arthur Fontijn, Rensselear Polytechnic Institute, Troy, NY (New Start)
1500		Break

Topic: Metalized Propellants

1530	40	BEHAVIOR OF ALUMINUM IN COMBUSTION OF SOLID ROCKET PROPELLANTS. Edward W Price, Robert K Sigman, Georgia Institute of Technology, Atlanta, GA
1600	41	DETERMINATION OF THE COMBUSTION MECHANISMS OF ALUMINIZED PROPELLANTS. John R Osborn and Robert L Glick, Purdue University, West Lafayette, IN
1630	42	AERODYNAMIC DROPLET BREAKUP. James E Craig and Robert G Oeding, Spectron Development Laboratory, Costa Mesa, CA
1700	43	EFFECT OF ACCELERATION ON METALIZED COMPOSITE PROPELLANTS. John R Osborn , Purdue University, West Lafayette, IN
1730		ADJOURN SESSION AND MEETING

ROCKET MOTOR AEROACOUSTICS

Warren C. Strahle
Georgia Institute of Technology
Atlanta, Georgia

Rocket motor combustion chamber pressure fluctuations are a source of rocket motor vibration that currently escapes predictability. The purpose of this program is to provide a theory, with experimental verification, that will enable prediction of the internal pressure and thrust fluctuation levels and spectra, given the turbulence structure and propellant impedance characteristics.

Figure 1 illustrates the physics involved if one observes the pressure on the wall of a rocket chamber. The pressure consists of a broadband component, random in space and time, and a propagational acoustic component. Since the chamber acts as a filter for the acoustics, the acoustic component is strongest near natural mode frequencies. Moreover, since there is a difference between head and nozzle end pressures for acoustic modes, this is the pressure component which can give rise to the largest thrust oscillations. By measurement of interior velocity fluctuations of the turbulence and use of aeroacoustics theory, agreement is sought between measured and predicted pressure, primarily with the acoustic component.

Figure 2 shows agreement between theory and experiment for one of two experimental configurations employed in cold flow. Shown is the theoretical calculation of the acoustic component of pressure, given turbulence data as the input. The experimental spectrum is primarily acoustic in nature, but has a broadband component.

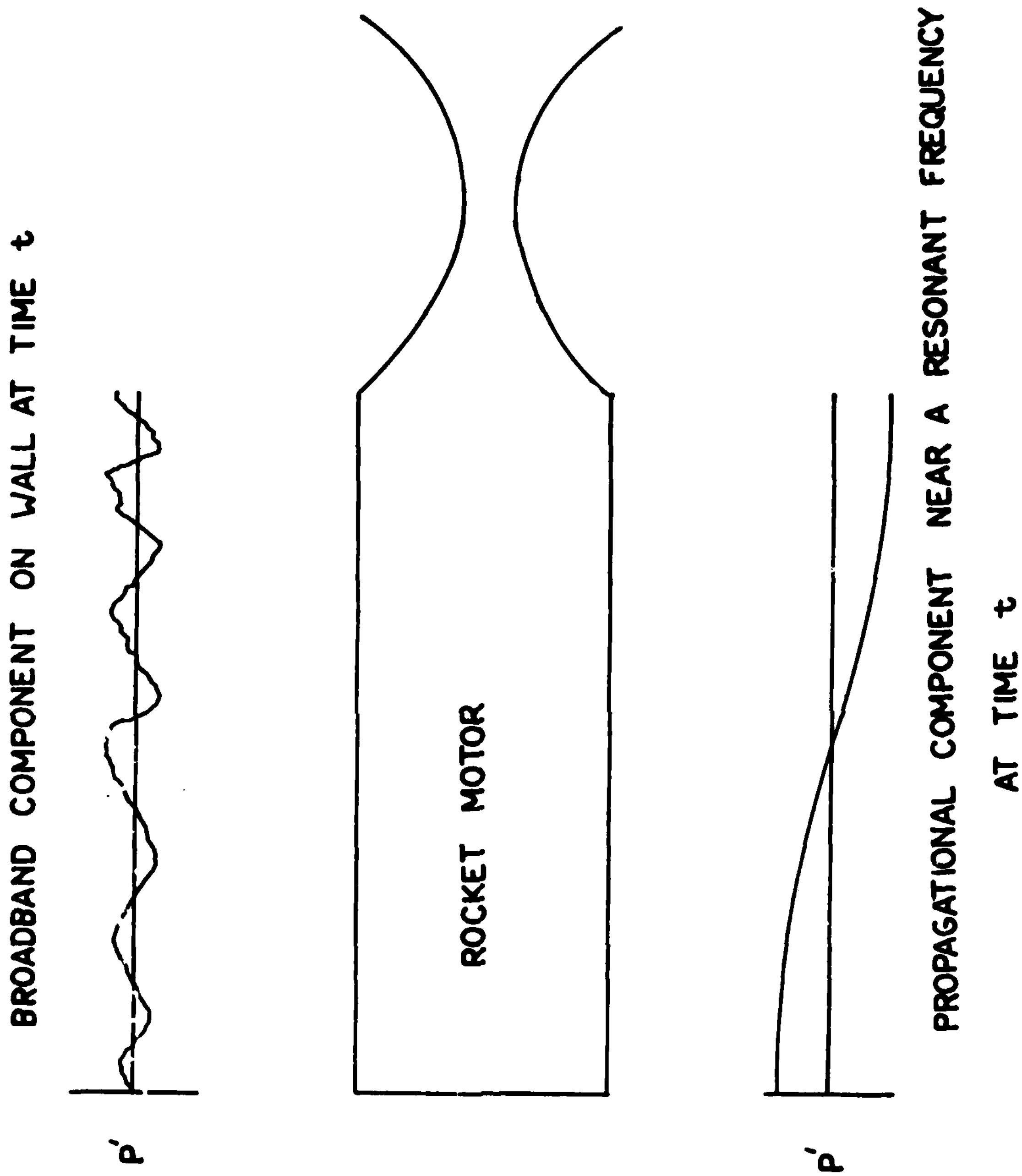

BROADBAND COMPONENT ON WALL AT TIME t
ROCKET MOTOR
PROPAGATIONAL COMPONENT NEAR A RESONANT FREQUENCY
AT TIME t
p'
p'

FIGURE 1

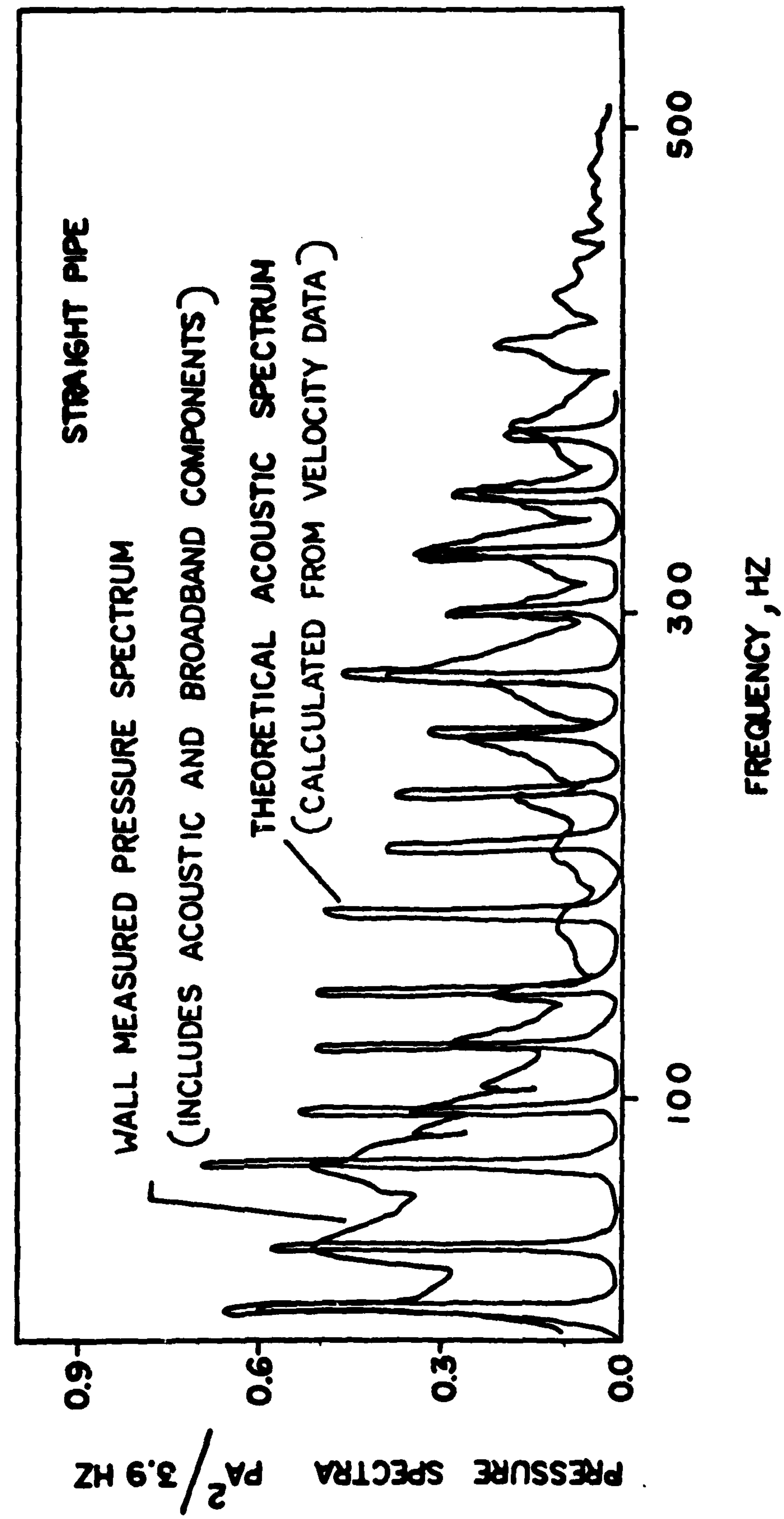

STRAIGHT PIPE
WALL MEASURED PRESSURE SPECTRUM
(INCLUDES ACOUSTIC AND BROADBAND COMPONENTS)
THEORETICAL ACOUSTIC SPECTRUM
(CALCULATED FROM VELOCITY DATA)
PRESSURE SPECTRA PA^2/3.9 HZ
0.0
0.3
0.6
0.9
100
300
500
FREQUENCY, HZ

FIGURE 2

Coupling Between Velocity Oscillations and Solid Propellant Combustion*

R. S. Brown, P. G. Willoughby, and R. C. Waugh
Chemical Systems Division/United Technologies

The dynamic coupling between velocity oscillations and the combustion process is a significant factor in determining the acoustic stability of a solid propellant rocket motor. A review of laboratory and motor test data reveals that currently modeling methods do not consider the detailed fluid mechanics involved in velocity coupling and are thereby quantitatively inadequate. Nonlinear wave behavior and changes in mean pressure have been used to formulate a qualitative heuristic model, but there is no mechanistically sound basis for quantitatively characterizing this coupling. Also, a review of studies on flow fields in chambers and on acoustics in ducts suggests that this coupling includes the effects of acoustic disturbances on turbulence in flows with high surface transpiration rates, acoustic streaming in the presence of combustion, and unsteady heterogeneous combustion processes. These processes involve fluid-dynamic and combustion-related phenomena that in themselves have not been studied qualitatively.

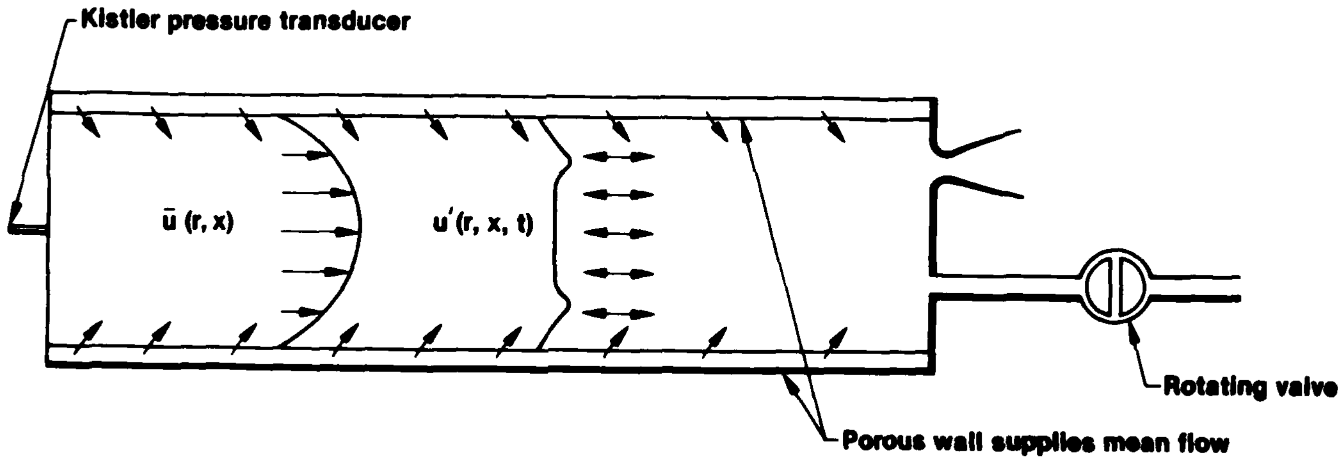
The objective of this continuation program is to investigate the interaction of unsteady oscillatory flow phenomena with the propellant combustion processes. Initial experiments are directed toward measuring the effect of acoustic velocity on the radial and axial profiles of the time average velocity, on the turbulence, and on the surface heat flux. To make these measurements, a cold flow apparatus, which is shown schematically in Figure 1, is being constructed to simulate the internal flow field in the combustor. Nitrogen flowing through large porous tubes simulates the flow of gas from the propellant surface. The overall length and nozzle throat diameter can be adjusted to permit the investigation of the effects of variations in the propellant burning rate and motor length-to-diameter ratio. A rotating valve at the nozzle exhaust plane provides a means of generating acoustic oscillations at a controlled frequency. Specific experimental studies address the effect of acoustic disturbances on turbulence profiles and surface heat flux as indicated in Figure 2. The effects of motor length, surface Mach number, and amplitude and frequency of the acoustic oscillations are the primary variables. The specific test conditions and interpretation of the results are closely coordinated with Princeton Combustion Research Laboratories, which is conducting analytical studies on this problem.

*Contract F49620-81-C-0027.

Figure 1

VELOCITY COUPLING WITH SOLID PROPELLANT COMBUSTION

APPROACH



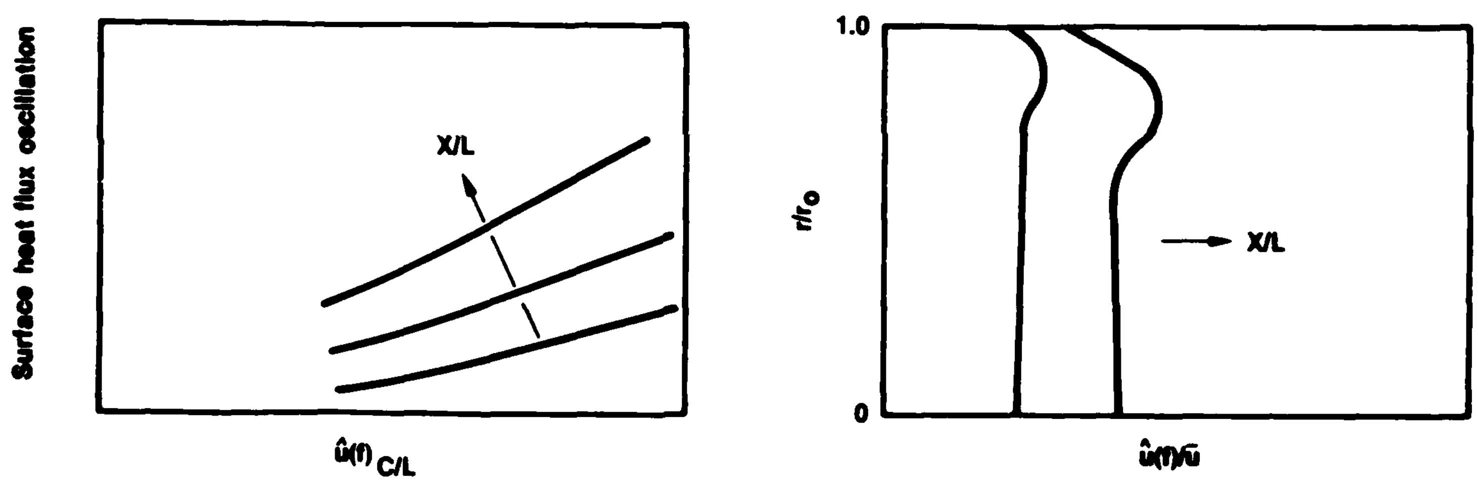
- Schematic of cold flow apparatus
- Objective

  Investigate:
  - Acoustic boundary layer
  - Turbulence generation
  - Vortex-boundary interaction

Figure 2

VELOCITY COUPLING WITH SOLID PROPELLANT COMBUSTION

ANTICIPATED RESULTS



- **Status:**
  Apparatus currently under construction

INTERNAL FLOW FIELDS & VELOCITY COUPLING

Moshe Ben-Reuven and Martin Summerfield

Princeton Combustion Research Laboratories, Inc., Princeton, N.J.

Several potential mechanisms of velocity-coupled instability in interior-burning solid propellant motors are investigated. These include, in particular: the effect of extended combustion in the coreflow, acoustic/wall-layer interactions, and turbulence/wall-layer interactions. The approach, as shown in Fig. 1, involves two major steps: (1) Obtain qualitative insights into the physical interactions involved in each of the aforementioned mechanisms, through order of magnitude estimates and linearized perturbation analyses. (2) Those mechanisms which show relevance to solid rocket instability (by demonstration of plausibility of dynamic coupling) will be subjected to more detailed numerical analysis. The present research is unique in that none of foregoing mechanisms was systematically investigated in conjunction with nonlinear combustion instability. It should be emphasized that aside from the direct application to combustion instability in rockets, this study is expected to contribute to basic research in acoustics and fluid dynamics, as implied by the remainder of this discussion.

The mechanism of nonlinear "acoustic streaming" or acoustic/viscous layer interaction is the subject of the present discussion. Some of the preliminary results are summarized in Fig. 2. Certain basic aspects of this phenomenon were theoretically investigated by Moore (1951), Lighthill (1954), C.C. Lin (1958), and others, as regards an impervious flat plate, in incompressible flow. Illingworth (1958) extended the linearized analysis to include effects of compressibility (to first order). Two important observations can be made: (1) The flow field in the wall layer is modified in the mean, by the appearence of a steady (or "DC") component, due to both viscous and convective transport, and hence requires second order analysis. (2) Oscillatory heat transfer and shear stress terms in the layer are due to viscous forces, obtainable by first order analysis. The compressible-flow analytical results derived by Illingworth for the surface heat transfer perturbation are of particular interest, as shown in Figs. 2a, b, where the amplitude and phase of the surface heat transfer perturbation are plotted against Strouhal number, (S) and frequency, respectively, with Mach number and pressure as parameters.

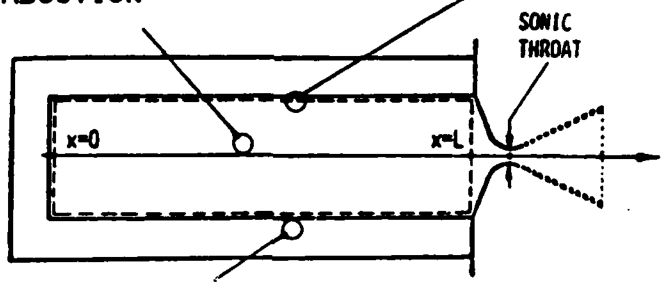
This linearized analysis is currently extended to incorporate mass injection at the wall (as indicated by Lam and Rott, 1960) and channel flow effects. The preliminary results strongly imply the relevance of acoustic/wall-layer interaction to velocity coupled combustion instability.

APPROACH: COOPERATIVE VELOCITY-COUPLING INSTABILITY RESEARCH PROGRAM

CONTRIBUTIONS TO CHAMBER DYNAMICS:

- MEAN FLOW
- DEVELOPING TURBULENT FLOWFIELD
- ACOUSTIC MOTIONS
- RESIDUAL COMBUSTION

- VISCOUS SUBLAYER WITH PRIMARY COMBUSTION



- SOLID PROPELLANT: ○ THERMAL WAVE RELAXATION
  ○ THERMOPHYSICAL, CHEMICAL PROPERTIES

THEORETICAL (PCRL)

- LITERATURE REVIEW
- EVALUATION OF VARIOUS V.C. MECHANISMS*
- DETAILED NUMERICAL ANALYSIS

EXPERIMENTAL (CSD/UTC)

- LITERATURE REVIEW
- COLD FLOW TESTS
- 2-D WINDOW MOTOR FIRINGS

INTERACTION:

- PRESSURE HISTORIES, VELOCITY PROFILES, TURBULENCE INTENSITIES, SURFACE HEAT TRANSFER, COMBUSTION BEHAVIOR
- COLD FLOW SIMULATION, NONSTEADY COMBUSTION SIMULATION, SUGGESTED MEASUREMENTS TO SUPPLEMENT THEORY

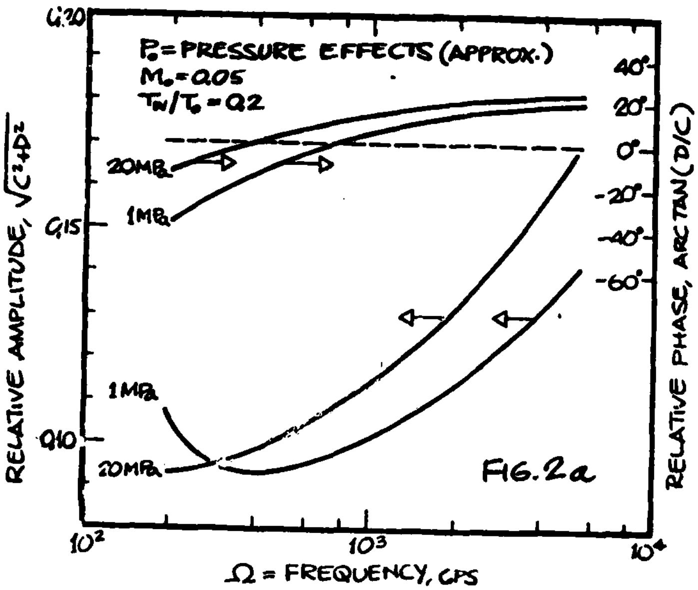
FIGURE 1.

*ACOUSTIC STREAMING; DYNAMIC EROSION; VORTEX/WALL LAYER INTERACTION, CORE-COMBUSTION COUPLING; OTHERS...

ACCOMPLISHMENTS:

ACOUSTICS/WALL-LAYER INTERACTION.

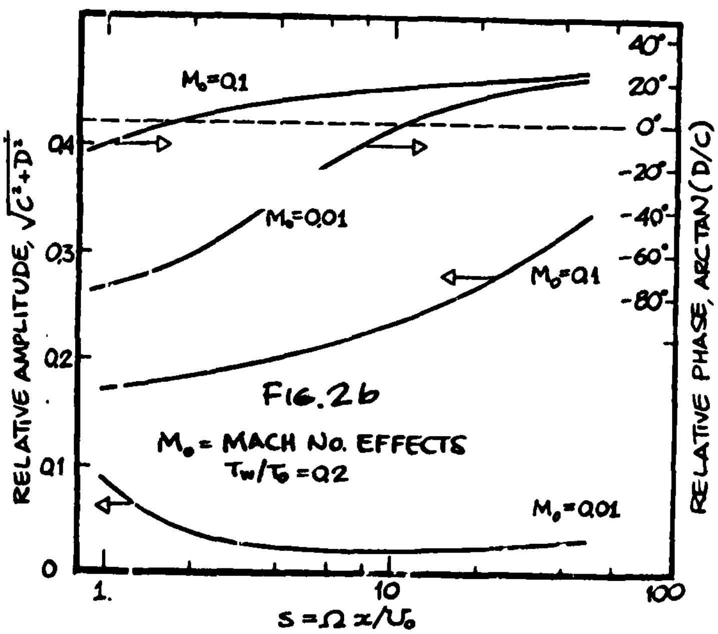
CALCULATED SURFACE HEAT TRANSFER PERTURBATION:



$$q_s' = \dot{q}_w/\dot{q}_{ws} - 1 = \varepsilon e^{i(\Omega t - M_o S)}(C + iD)$$

$$C, D = f\left(\frac{T_w}{T_o}, M_o; S\right)$$

AFTER ILLINGWORTH (1958), LINEARIZED STUDY (COMPRESSIBLE FLOW, FLAT PLATE, FIRST ORDER).



CONCLUSION:

AMPLITUDE ~ O(Mo) AND PHASE ANGLE SHOW RELEVANCE TO COMBUSTION INSTABILITY PROBLEM

FIGURE 2

Investigation of the Velocity and Pressure Coupled Admittances of Aluminized and Nonaluminized Propellants

Ben T. Zinn and Brady R. Daniel

Aerospace Engineering, Georgia Institute of Technology
Atlanta, Ga. 30332

This research program is concerned with: (1) development of reliable experimental techniques for the determination of the admittances of solid propellants under different oscillatory flow conditions; (2) development of diagnostic capabilities for the determination of the structure of the oscillatory flow field in the region adjacent to the burning solid propellant; (3) utilization of the measured data to develop an understanding of the mechanisms that control the unsteady response of different solid propellants; and (4) determination of the response characteristics of different solid propellants under different oscillatory flow conditions.

Answers to the above questions are pursued using two modified impedance tube setups. The first setup, developed earlier under this program, is capable of determining the pressure response of aluminized and nonaluminized solid propellants under different operating conditions. The second, recently developed, impedance tube has been designed for the simultaneous determination of (1) the velocity coupled response of the tested solid propellant and (2) the structure of the flow field next to the propellant surface. An isometric sketch of the new impedance tube is shown in Fig. 1. The driver propellant at one end provides the needed flow of hot gases past the test propellants which are placed on opposite walls at a preselected location. An acoustic driver at the other end is used to setup a standing wave of a desired frequency in the tube and a stepping motor to keep the test propellant surfaces flush with the adjacent walls. During a test, the driver is turned on, the propellants ignited simultaneously and the structure of the resulting standing wave in the tube is measured using pressure transducers distributed along the tube's wall. The measured data are then input into a computer program that determines the velocity coupled admittance of the test propellants.

To understand the mechanisms that control the characteristics of the measured propellant admittances, the structure of the flow field adjacent to the propellant surface will be measured simultaneously with the admittance measurements. Efforts are underway to develop diagnostic capabilities for obtaining the desired data. Initial efforts focus on the use of LDV to measure the velocity field and subsequent efforts will proceed to investigate the temperature, particulates and, possibly, concentration fields.

The approach utilized in this study to investigate the unsteady response of solid propellants is unique in the sense that it would possess capabilities for <u>simultaneous</u> measurements of the propellant response and the structure of the oscillatory flow field next to the propellant surface under different operating conditions. Analysis of these data is expected to isolate the factors which exert the greatest influence upon the burning propellant, provide data for guiding the development of theoretical models, and develop information that should help design stable solid rocket motors.

In a recently completed study, the impedance tube was utilized to investigate the effect of aluminum addition upon the propellant driving and the associated gas phase losses. Three similar propellants having 0, 5 and 18 percent aluminum were tested and the results are compared in Fig. 2 where the frequency dependences of Y_r, the real part of the admittance, and G, the gas phase losses, are plotted. Interestingly, these results show that (1) aluminum addition generally increases <u>both</u> the propellant driving and associated gas phase damping; (2) aluminum addition <u>shifts</u> the frequency at which maximum driving occurs; and (3) the response curve may have more than one peak. While these results are under further study, they indicate that aluminum addition may, under certain conditions, destabilize rocket motors.

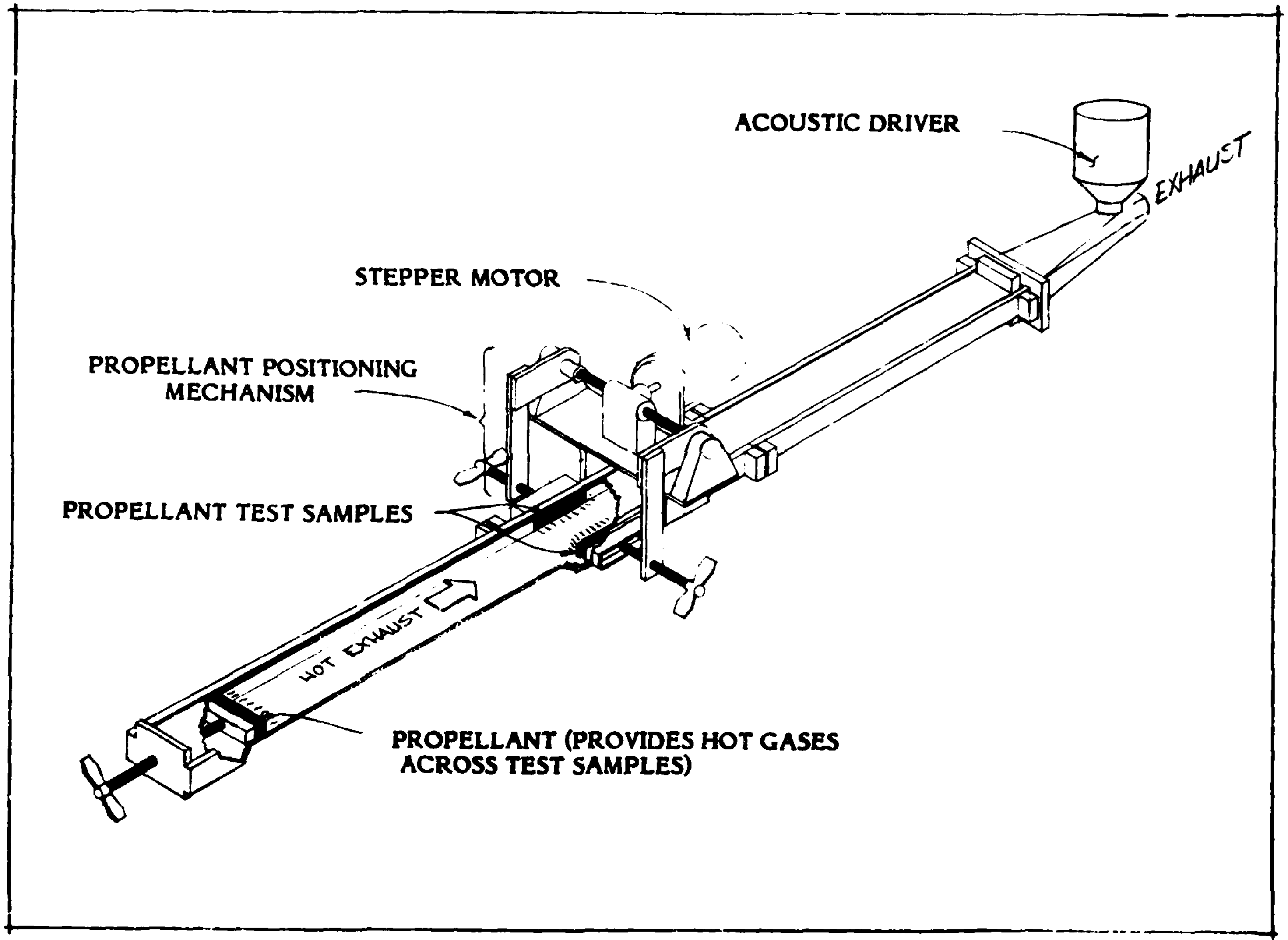


Figure 1. Modified Impedance Tube for Velocity Coupling Response and Diagnostics Measurements.

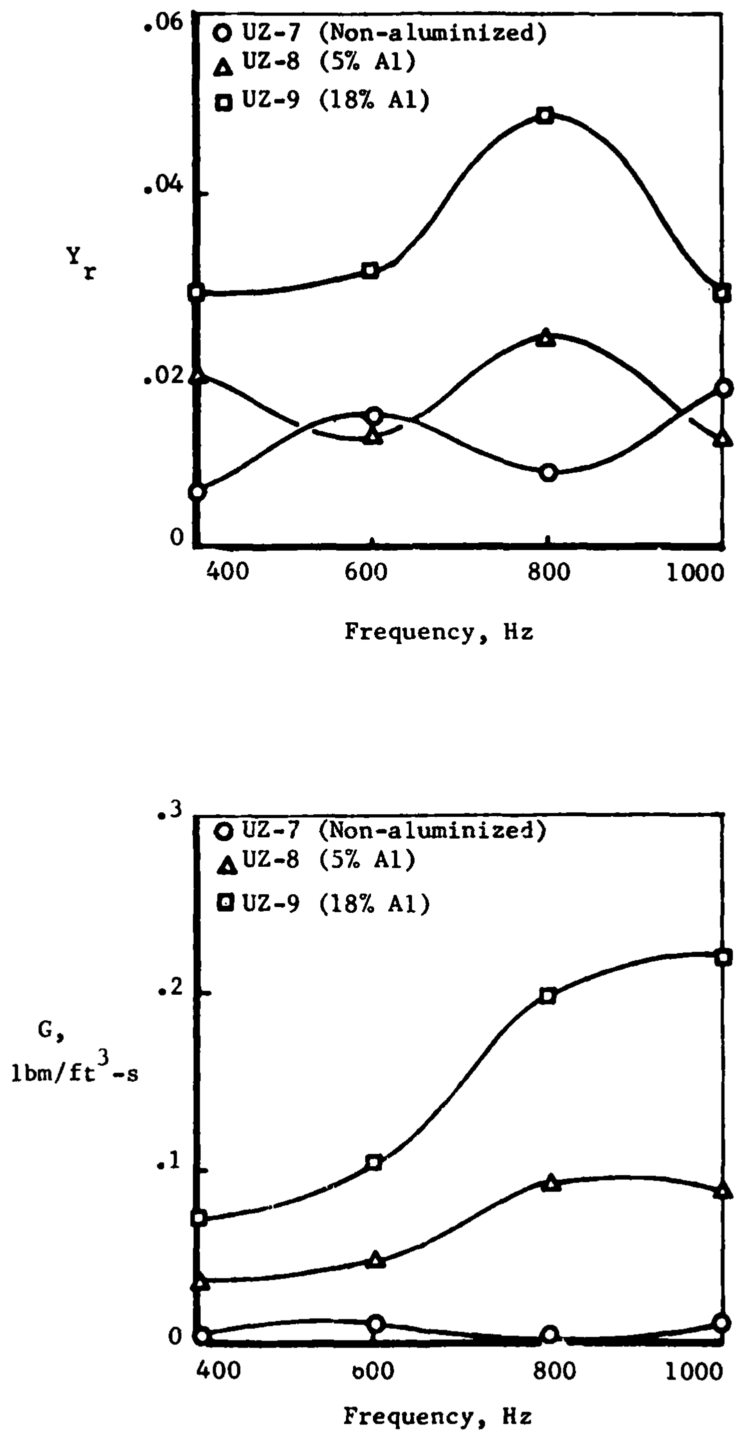


Figure 2. Dependence of Propellant Driving, Y_r, and Associated Gas Phase Losses, G, upon Frequency and Propellant Aluminum Content.

NONLINEAR COMBUSTION MODELING

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The objective of the present research program is to further our understanding of the physical mechanisms which control the initiation and severity of nonlinear combustion instability in solid rocket motors. The ultimate goal of this work is the development of a comprehensive analytical model capable of predicting the relative nonlinear stability of solid rocket motor designs.

The present approach is outlined in Figure 1. Mathematical models of the known, operative, physical mechanisms governing nonlinear wave propagation in two phase media and the nonlinear transient combustion response of the propellant, have been formulated as a coupled set of partial differential equations. These equations are solved numerically using appropriate finite difference techniques. The analytical solutions are then compared to data obtained from motor firings to determine their ability to predict the phenomena which have been observed. Detailed examination of the numerical solutions provides new insight into the nature and causes of nonlinear combustion instability.

The comprehensive physical model and advanced numerical techniques used in the current approach make it uniquely capable of treating multiple shock wave, triggered, instabilities in variable cross-sectional area, reduced smoke tactical motors; currently the most prevalent form of nonlinear instability. Previous methods all have various deficiencies which preclude their ability to analyze this problem.

The primary accomplishments in the past year are as follows. The ability of the Lax Wendroff + Hybrid + Artificial Compression numerical scheme to accurately treat multiple shock wave propagation in variable area chambers was verified. A large number of solutions were obtained which demonstrated that the limiting amplitude attained by an instability is independent of the characteristics of the initiating disturbance. Two different ad hoc velocity coupling models were developed. From solutions obtained with these models it was concluded that: quasi-steady gas phase, homogeneous solid phase, velocity coupling models are not capable of producing strong nonlinear effects at realistic response function values; nonlinear oscillations in solid rocket motors are a complex combination of traveling and standing waves; observed modulations in limit cycles are a result of the phase angles between the pressure, velocity, and burning rate oscillations being non-stationary in time.

Figure 2 presents results which demonstrate the ability of the present analysis to predict: triggering at a finite disturbance amplitude; DC pressure shifts modulated amplitude limit cycles; and strongly nonlinear waveforms. All of these phenomena have been observed in actual solid rocket motor firings.

An a priori method for predicting the pulse characteristics produced by a variety of laboratory pulsers has also been developed. Comparisons with experimental pulse measurements show excellent agreement.

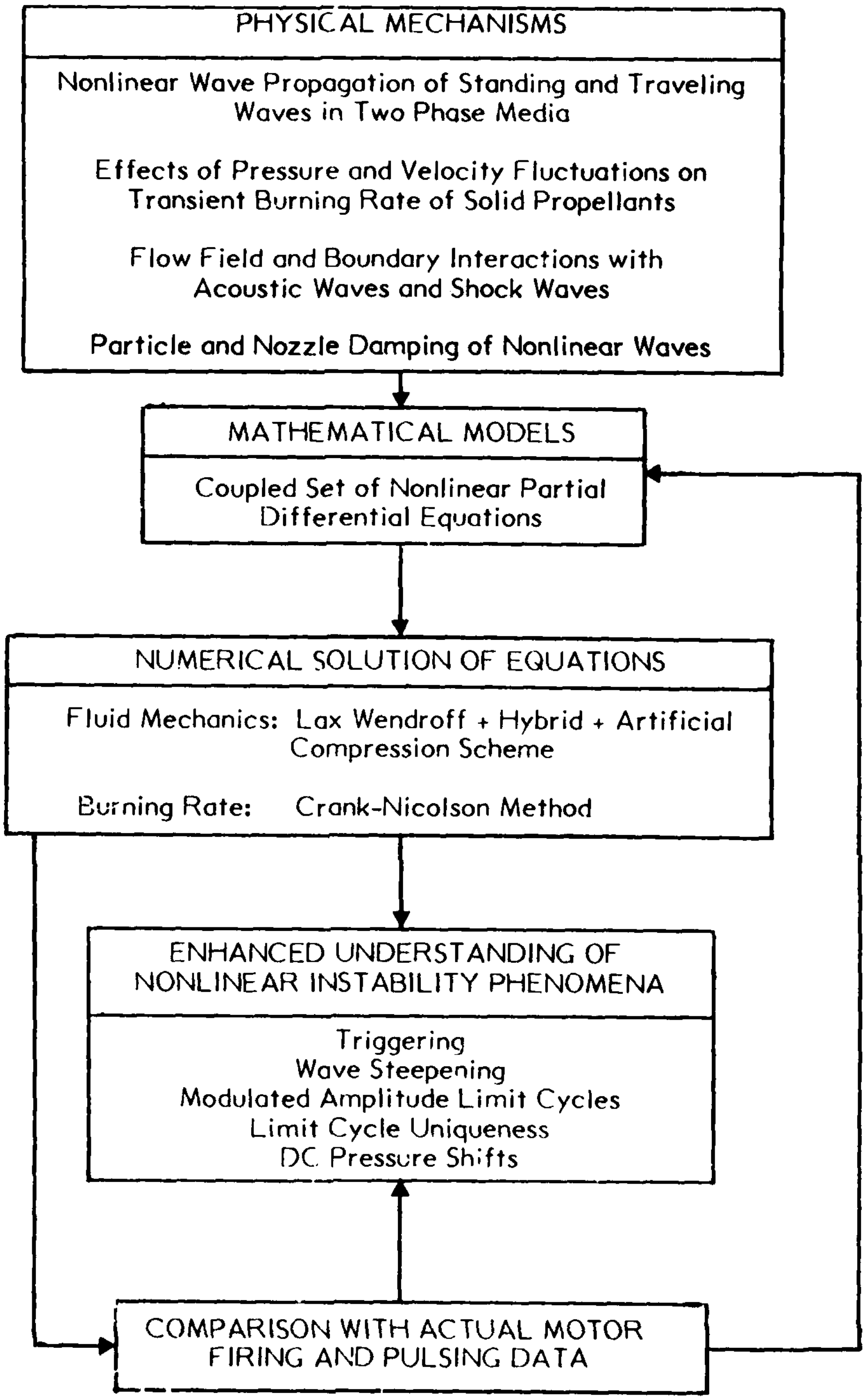

FIGURE 1. OUTLINE OF SCIENTIFIC APPROACH

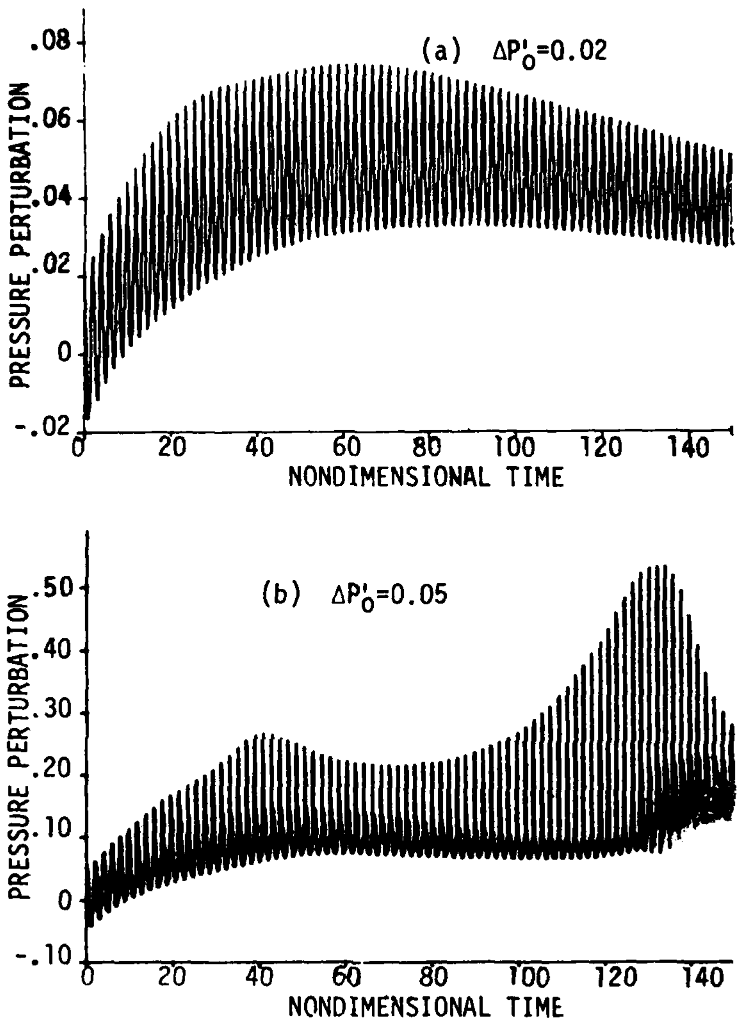

FIGURE 2. Numerical Simulation of Nonlinear Instability Demonstrating Triggering at Finite Amplitude, DC Pressure Shift, Modulated Amplitude and Highly Nonlinear Waveforms.

OVERVIEW: AFOSR RESEARCH INTERESTS IN ROCKET PROPULSION

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Powerful motivations exist for research on propulsion and reacting flow processes. Many of the phenomena that occur have not been explained adequately in terms of physical models. In this sense, propulsion and reacting flow processes represent scientific challenges suggesting that research will advance areas such as the physicochemical bases for new energetic materials, methods of releasing energy, exhaust plume prediction, and insuring combustion stability. Achieving mechanistic understandings which are consistent over a broad range of a categories is a continuing effort. Data relating to items such as global kinetics, intermediate species, and surface structures obtained in one regime probably do not apply in another. Thus part of the research is based on the situation that we often have no alternative but to extrapolate from the available data bases.

For many situations, the literature contains a sufficient selection of physical property values that a set can be found to produce correlations using calculated results from ill-posed models. As part of this presentation, the usefulness of such parametric-fitted type models is questioned in view of the scientific goals of achieving a more complete understanding. In many cases, the research community is better served by authors pointing out those processes responsible for the greatest uncertainity in the calculated trends. Such explicit statements of limitations stimulate interdisciplinary responses and participation, a notion consistent with the goals of this meeting.

The presention is intended to stimulate thinking on the more challenging research goals. During the next year, opportunities exist for bold scientific approaches. The format of this meeting provides insights into numerous areas of interest, e.g., presentations by Air Force personnel, appendices in this document, and most importantly direct contact with Air Force personnel responsible for specific areas. The table includes examples of research opportunities. Of course, our interests are not limited by the tabulated items; the most important research topics and approaches resulted from the independent thinking of the principal investigators.

The long-term funding and flexible work statements of AFOSR are intended to provide conditions conducive to undertaking the more challenging problems using techniques at the forefront of technology. Propulsion research is endowed with a number of eternal goals, i.e. higher energy, higher reliablity, lower cost, and more complex mission requirements. Thus research directed at making evolutionary progress, even to mature propulsion systems, will have payoffs. Also, research to eliminate interactions (e.g., combustion instablity, ambient temperature constraints) which limit performance is necessary. However, the challenge in energy conversion research is to provide direction for achieving higher energy and new power sources. During FY82, the activities in this last category are disproportionately small As part of the FY83 initiatives, new research is being planned in anticipation of future Air Force space missions which will require substantially higher power and more efficient propulsion for orbit raising and maneuvering. Thus, particular interest is expressed in nonconventional propulsion and power means for space. Some specifics on this initiative are given in Appendix 3. Also, the requirements to deliver larger pay loads to low earth orbit and the plans for greater use of space present possibilities.

Table

EXAMPLES OF RESEARCH OPPORTUNITIES

COMBUSTION

O ACCELERATE METAL FUEL COMBUSTION FOR AIR BREATHING SYSTEMS
  + INCORPORATION OF RESULTS OF CURRENT KINETICS STUDIES
  + EXPLOIT ADVANCED INSTRUMENTATION TO LABORATORY SCALE EXPERIMENTS

O CONTROL COMBUSTION OF MONOPROPELLANT (E.G. NITRAMINE) COMBUSTION
  + CONTRIBUTION OF LIQUID LAYER DECOMPOSITION PROCESSES
  + REACTION ACCELERATION AND CONTROL

O INCREASE FLOW AND METAL COMBUSTION EFFICIENIES FOR CONVENTIONAL ROCKETS
  + MECHANISMS OF METAL/METAL OXIDE AGGLOMERATE FORMATION
  + PROCESSESS LEADING TO SUBMICRON METAL OXIDE PARTICLES

COMBUSTION STABILITY

O DIRECT MEASURMENT OF ACOUSTIC ADMITTANCE
  + POSITION COUPLED LDV SYSTEM AND TIME SERIES ANALYSIS
  + DYNAMIC SURFACE TRACKING

O SUPPRESSION OF COMBUSTION INSTABILITIES
  + MECHANISM OF PARTICULATE ADDITIVES
  + INFLUENCE OF CHAMBER DESIGN AND DISSIPATORS

PROPULSION

O ADDRESS ENABLING TECHNOLOGIES AND CRITICAL ISSUES ASSOCIATED WITH:
  + ADVANCED CHEMICAL PROPELLANTS
  + BEAMED ENERGY APPROACHES
  + ELECTRIC THRUSTERS
  + ELECTROMAGNETIC MASS ACCELERATORS
  + NUCLEAR PROPULSION

PROPELLANTS

O HIGHER ENERGY INGREDIENTS IN TERMS OF PROPULSION SYSTEM REQUIREMENTS
  + IDENTIFY TECHNOLOGICAL BARRIERS REQUIRING BASIC RESEARCH
  + MECHANISMS LEADING TO UNSATISFACTORY PROPERTIES
  + CHARACTERIZE INGREDIENTS IN TERMS OF MOLECULAR STRUCTURE
  + MORE ENERGETIC AND LESS SENSITIVE BINDERS
  + BINDERS TO PRODUCE IMPROVED PHYSICAL PROPERTIES AND AGING
  + NEW RESEARCH TOOLS,E.G. MOLECULAR DYNAMICS MODELS, MODERN INSTRUMENTS

DIAGNOSTICS OF REACTING MEDIA

O ULTRA-HIGH SPEED REACTION DETECTION
  + KINETICS OF CRYSTAL PHASE CHANGE
  + LIQUID LAYER DECOMPOSITION

O QUANTITATIVE MEASUREMENTS IN REACTING TWO PHASE FLOWS
  + 2-D CONCENTRATIONS, TEMPERATURES, AND VELOCITIES OF BOTH PHASES
  + 2-D MIXING PARAMETERS AT SHEAR FLOW INTERFACES

SOLID PROPELLANT AIRBREATHING COMBUSTION RESEARCH

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This project has had split purposes during the year as an external/base burning effort was completed and a new project on solid fueled ramjet flame stabilization was begun. The base burning work culminated with extremely high performance results and clearly showed that a 6.2 effort would be desirable. Initial work on the SFRJ project has consisted of wind tunnel design and modification and laser diagnostics set-up and checkout, with initial turbulence modelling being conducted on the analytical side.

In Fig. 1a, the wind tunnel test section for the Mach 3 external/base burning tests is shown. Over the past 4 years the tests run have included a) cold flow tests with base injection, b) base burning tests with subsonic base and radial injection, c) combined base and external burning tests using supersonic radial injection, d) base burning tests with diluted fuel injection and e) a combination of preburning with base burning. In Fig. 2a the results of the final series of tests with preburning is shown. Exceptionally high performance is shown, as compared with cold gas base burning.

In Fig. 1b, the SFRJ flameholding region is shown, which is the region of interest in this program. Laser diagnostics will be run in cold and hot flows for velocity (mean and fluctuating), concentration and temperature. Two facilities, one cold and one hot, will be or are being constructed. Analytical modelling at the second order closure level for this turbulent flow has begun. Typical kinds of tests for this modelling are shown in Fig. 2b, where the shear stress computed by the k-ϵ method is compared with experiment (others') in cold flow near the reattachment point. A crucial issue with this flow is accurate computation, in order to have predictability for flame stability limits and fuel regression rate.

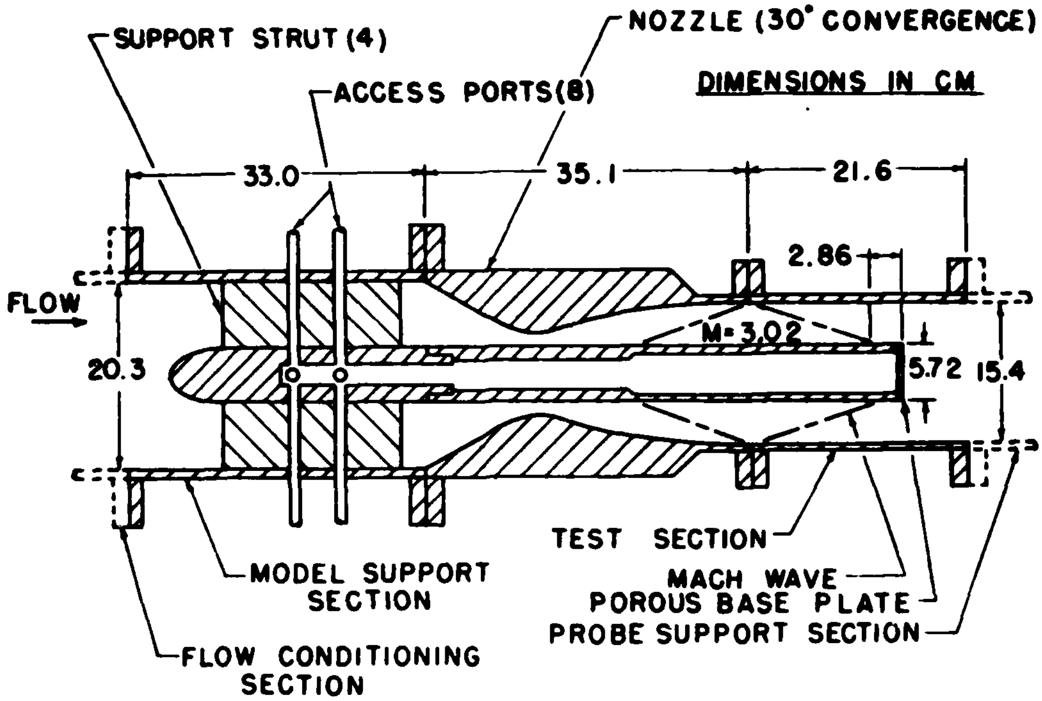

Figure 1a. External/base burning wind tunnel test section.

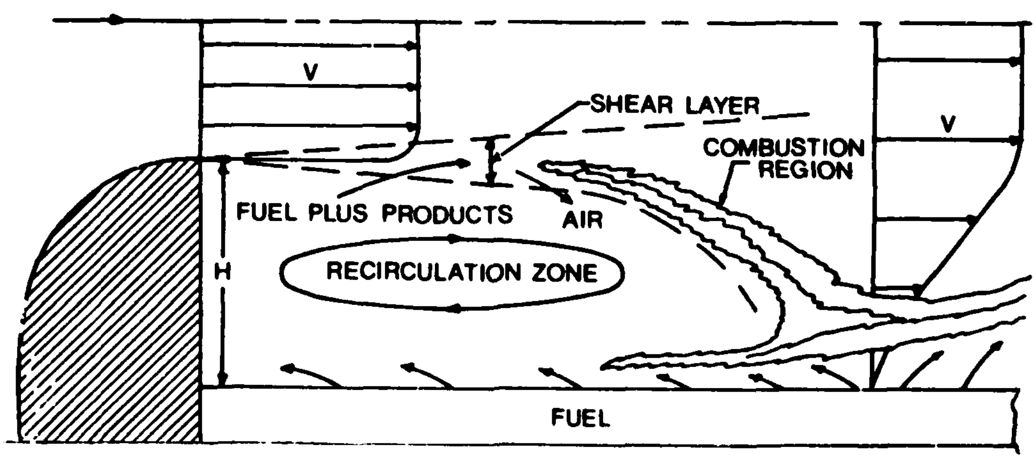

Figure 1b. SFRJ flow field in the stabilization region.

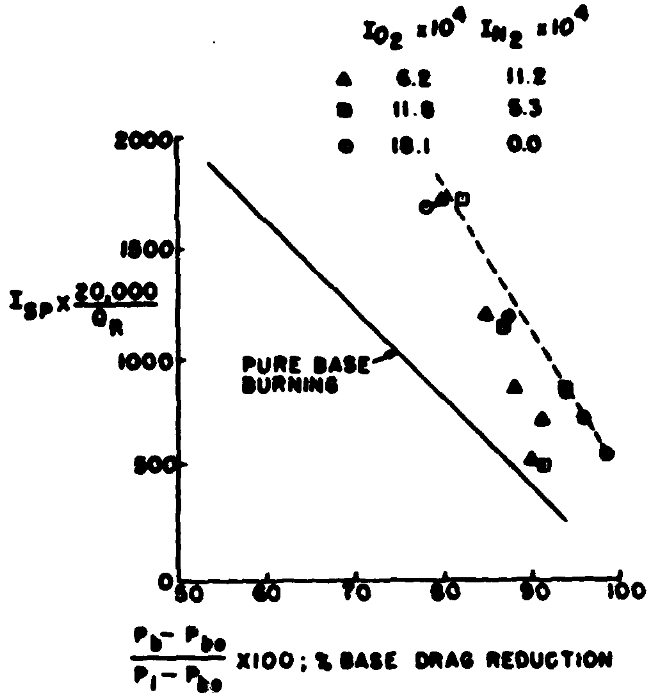

Figure 2a. Base burning results with preburning.

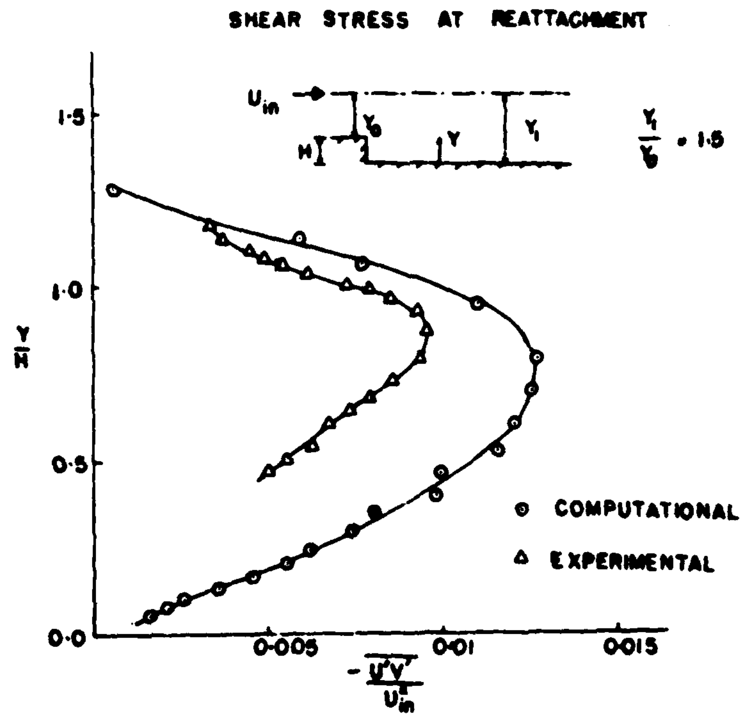

Figure 2b. Comparison of shear stress at reattachment - experiment vs k-ε theory.

FUEL-RICH SOLID PROPELLANT BORON COMBUSTION

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Atlantic Research Corporation
Alexandria, Virginia

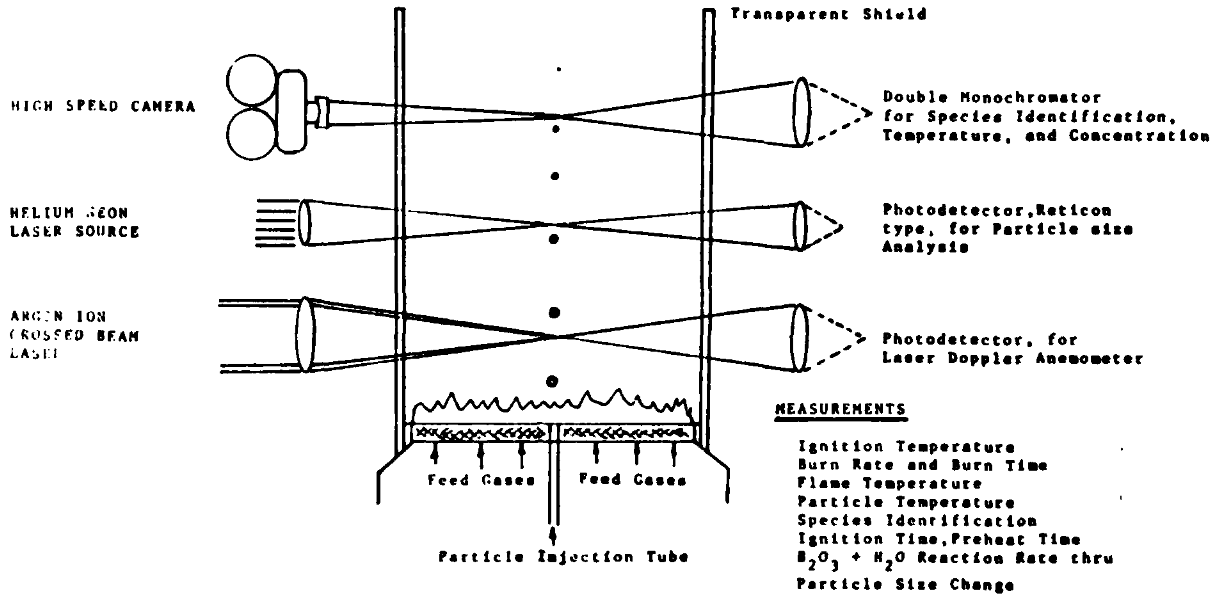
Boron is a particularly attractive ingredient for airbreathing missile fuels due to its high gravimetric and volumetric heating values. For achievement of full potential, however, boron particles must ignite and burn completely within a very limited residence time. Since boron particles are generally initially coated with an oxide layer which inhibits combustion and since boron metal has an extremely high boiling point which necessitates surface burning subsequent to oxide removal, this can become difficult, and afterburning efficiency problems have been encountered with boron fuels. Ramburner combustor design optimization is particularly critical to achievement of high efficiency and definition of approaches to such optimization depends on good understanding of the phenomena involved in boron particle ignition and combustion. A thorough critical review of the literature in this area has revealed numerous knowledge gaps.

A multi-faceted effort involving interlocked analytical and experimental tasks is planned. A list of the major tasks appears on Page 3. Fundamental experiments aimed at quantifying kinetics of various reactions involved in boron ignition and combustion will provide data to be used in detailed models of these processes. These models will in turn be combined with mass, momentum, and energy balance equations to develop prediction procedures for ignition and flame stabilization of boron dust clouds in combustors and for prediction of fractional heat release in confined volumes. Additional experiments will be conducted to confirm these predictive tools. In addition, various chemical and physical techniques aimed at improving boron ignition and combustion processes will be tested. Finally, flame structures associated with consolidated boron grains will be examined and means of tailoring these structures to desired characteristics will be investigated.

At this point, the literature review has been completed. In addition, major modifications to the equation set used in analyzing boron single particle ignition have been made, with use of information obtained from the literature (particularly the Russian literature) and a revised computer code for prediction of critical ignition conditions and ignition delay times is essentially complete.

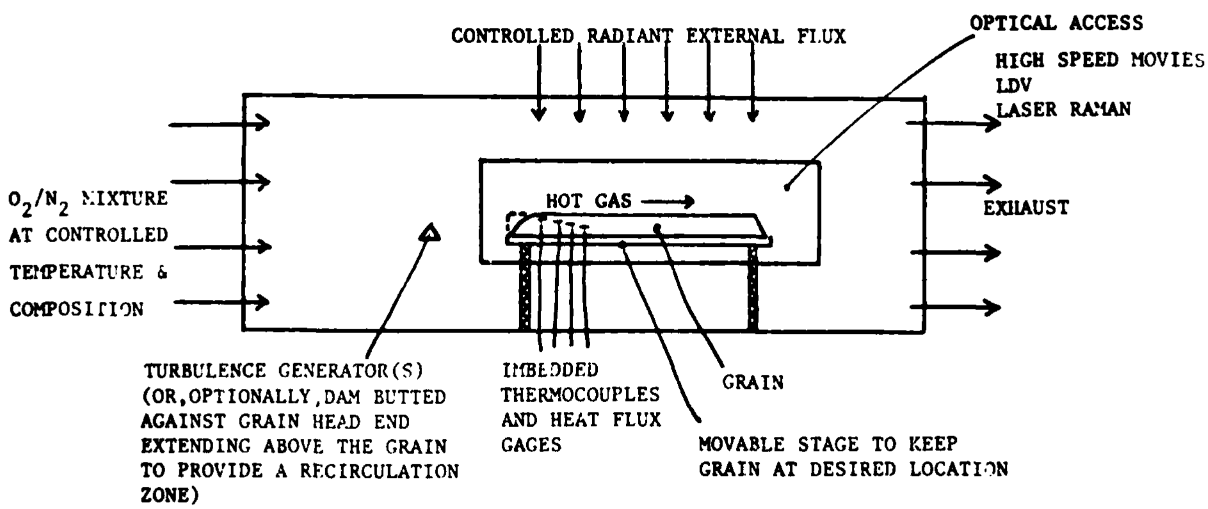
A completely revamped, highly modernized (particularly in terms of data acquisition) flat-flame burner facility (Page 2 - Top) has been constructed and experimental studies of single particle ignition and combustion are just beginning. Diagnostic methods include conventional chopped-frame photography, line scan image intensification, laser velocimetry and particle interferometry. Spectral observations of the oxide coating degradation are planned for the near future.

The mechanisms involved in the ablation of consolidated boron grains in a high temperature air crossflow and in subsequent combustion of material leaving the surface are not well understood. (In fact, even the nature of the products leaving the surface is not well defined.) It is thought that two factors of major importance are radiation heat feedback from particles burning in the mainstream to the surface and the nature of the flow and turbulence profiles near the surface. The apparatus sketched at the bottom of Page 2 will be used to study these effects and define at least qualitatively the important processes. Diagnostics will include high-speed photography, laser schlieren, LDV and laser raman spectroscopy for definition of the nature of products leaving the surface and processes occurring in the gas phase, while imbedded thermocouples and heat flux gages will be used to determine subsurface temperature profiles and heat feedback fluxes (radiative and non-radiative). Sampling probes may also be employed for definition of ablation products. Construction of this facility is currently under way.



SINGLE PARTICLE BORON IGNITION/COMBUSTION EXPERIMENT

(AND EXPERIMENT FOR STUDY OF $H_2O(g)$ + $B_2O_3(l)$ KINETICS)



CONSOLIDATED GRAIN COMBUSTION MECHANISM EXPERIMENT

• MAJOR TASKS PLANNED

(1) Conduct exhaustive critical review of domestic and foreign work on boron ignition/combustion phenomena.

(2) Extensively modify existing single particle boron ignition model, extending it to properly treat the effects of H_2O on particle ignition.

(3) Develop a mechanistically accurate model for boron particle combustion in the kinetics-controlled regime.

(4) Develop a boron cloud ignition model.

(5) Develop stirred reactor and directed-flow models of boron cloud combustion using unit models developed in above tasks.

(6) Evaluate feasibility of various approaches to measuring kinetics of $B(s) + O_2$, $B(s) + H_2O$, $B(s) + CO_2$.

(7) Define experiments to quantify problem of conversion of $HBO_2(g)$ to $B_2O_3(l)$.

(8) Experimentally study kinetics of $B_2O_3(l) + H_2O$, using flat-flame burner.

(9) Experimentally identify intermediates appearing in boron combustion.

(10) Use flat-flame burner techniques to obtain ignition and burn-time data for single boron particles in the 5 to 25 micron size range.

(11) Study conversion of boron in a CTRZ reactor.

(12) Investigate the flame structure associated with burning of a consolidated boron grain in an air crossflow.

(13) Experimentally evaluate the effects of boron ignition promoters.

(14) Experimentally study ignition delay times for boron dust clouds.

(15) Measure boron dust cloud flame speeds as functions of various parameters.

• ACCOMPLISHMENTS TO DATE

(1) Literature review completed and presented as a paper at the 18th JANNAF Combustion meeting.

(2) Single particle ignition modeling nearly complete.

(3) Flat-flame burner facility completed and single particle ignition/combustion testing initiated.

(4) Consolidated grain combustion mechanism test apparatus designed and under construction.

The Potential for Using Electromagnetic Energy to Supply Propulsion Energy

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Future Air Force space missions will require a broad range of thrustor capabilities. Although current systems will be adequate for many of these missions, some will require propulsive capabilities which are not currently available. The present research program is directed toward evaluating the potential of one concept which offers promise of filling this gap, namely, beamed energy. Primary emphasis is placed on identifying those issues most critical to the eventual implementation of beamed energy systems and finding methods for circumventing these issues.

Beamed energy propulsion includes a number of distinct scenarios as suggested in Fig. 1. The beam may be composed of laser, microwave, or concentrated solar energy. A laser beam may be generated by absorbing solar energy in a gas which is used to pump the laser. Similarly, laser energy may be obtained from a nuclear reactor via a nuclear-pumped laser, or from chemical or E-beam driven lasers. Solar energy may also be converted to electricity by means of solar cells and used to generate microwaves, or it may be used directly without an intermediate step. At present none of these methods possess a clear-cut advantage over the others even though the intermediate steps may contain substantial inefficiencies.

For any of these cases, the beam radiation is used to heat a working fluid which is then expanded through a nozzle to provide thrust. Details of the absorption process are also shown on Fig. 1. The incoming radiation passes through a window and into the working fluid where it is converted to random thermal working fluid where it is converted to random thermal energy. Wall cooling, absorption characteristics of the gas, and performance goals dictate that this energy be deposited in a hot inner zone with a cool buffer gas near the walls. The working fluid may be pure hydrogen or hydrogen seeded with materials designed to improve absorption or to protect the walls from thermal loads.

Some preliminary results of a one-dimensional model of the radiant energy absorption process are shown in Fig. 2. The energy deposition rate is controlled in large part by the absorptivity of the gas. As shown here, the absorptivity is a strong function of wavelength and in addition changes by some ten orders of magnitude over the temperature range of interest. Figure 2 also shows upper bounds on the primary losses which can occur in beamed energy engines. Performance estimates show that specific impulses between 800 and 2000 sec. are possible at thrust levels approaching 1000 n.

PRODUCTION OF THRUST FROM ELECTROMAGNETIC RADIATION

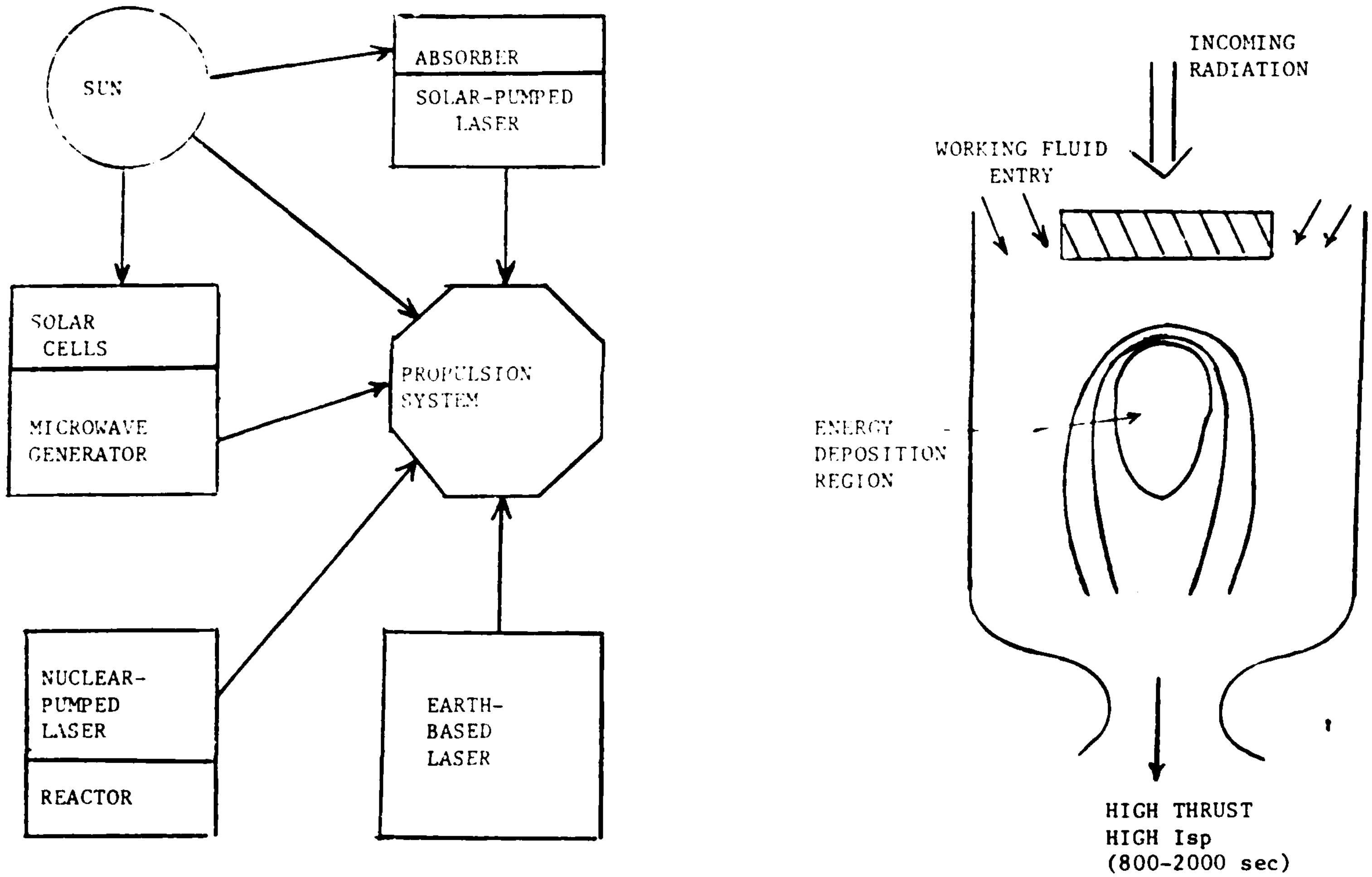

Fig. 1 Basic Issues and Main Features of Approach

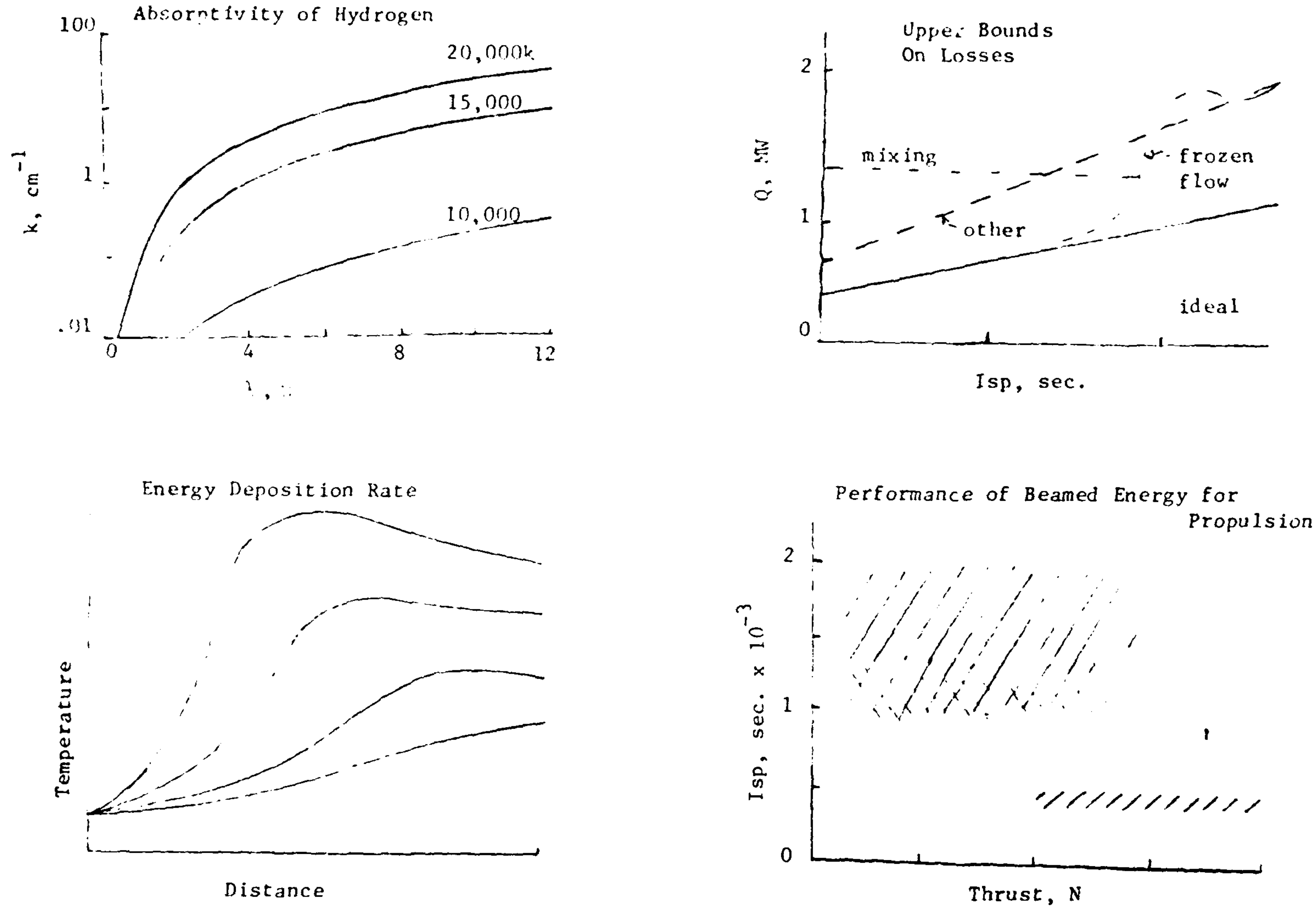

Fig. 2 Primary Accomplishments and Anticipated Results

ELECTROMAGNETIC ACCELERATION OF ROTATING CHARGES

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All versions of electromagnetic propulsion operate by applying a Lorentz body force to charges. This force is the resultant cross product of the charge velocity and the requisite magnetic field. The magnetic field can be externally induced or self-induced by the moving charges and the charges themselves are set in motion by means of an electric field. Magnetoplasmadynamic thrusters, rail guns, pulsed inductive thrusters and mass drivers among others all operate by the above principles. Previously, in order to utilize a gaseous propulsive fluid, the gas had to be at least partially ionized so that a charge velocity could be induced. Such ionization requires a large amount of electrical power and an expenditure of energy which is not recoverable. Mass drivers, which exhibit a high efficiency, utilize currents flowing in metallic conductors and avoid the ionization problem. If a gaseous propellant could be utilized in an electromagnetic propulsion scheme without the need for ionization, performance could be increased without the need for large amounts of electrical power.

One recently suggested method by which the electromagnetic acceleration of a nonionized gas could be obtained involves the use of atoms or molecules with a net neutral charge but possessing dipole moments. A rotating electric field can set dipole moments in rotation. The rotating dipoles each constitute two charges moving in opposite directions at any instant of time. If an alternating magnetic field is applied, the Lorentz body forces acting on both charges in the dipole are in the same direction and thrust is produced (Fig. 1). The dipole acceleration which is a function of dipole moment to mass ratio, rotation frequency and magnetic field strength can be calculated. This research will examine various physical processes which may effect the ideal performance of a rotating dipole thruster. These processes include collisional effects, dissociation, stray ionization and the technological ability to produce electric and magnetic fields of sufficiently high strength and frequency. In order to be a viable concept, a thrust density an order of magnitude greater than that obtainable with ion thrusters with a specific impulse of at least 1000 seconds is necessary. Figure 2 plots the region of attainable thrust density and specific impulse as predicted by a preliminary analysis for a rotating dipole thruster.

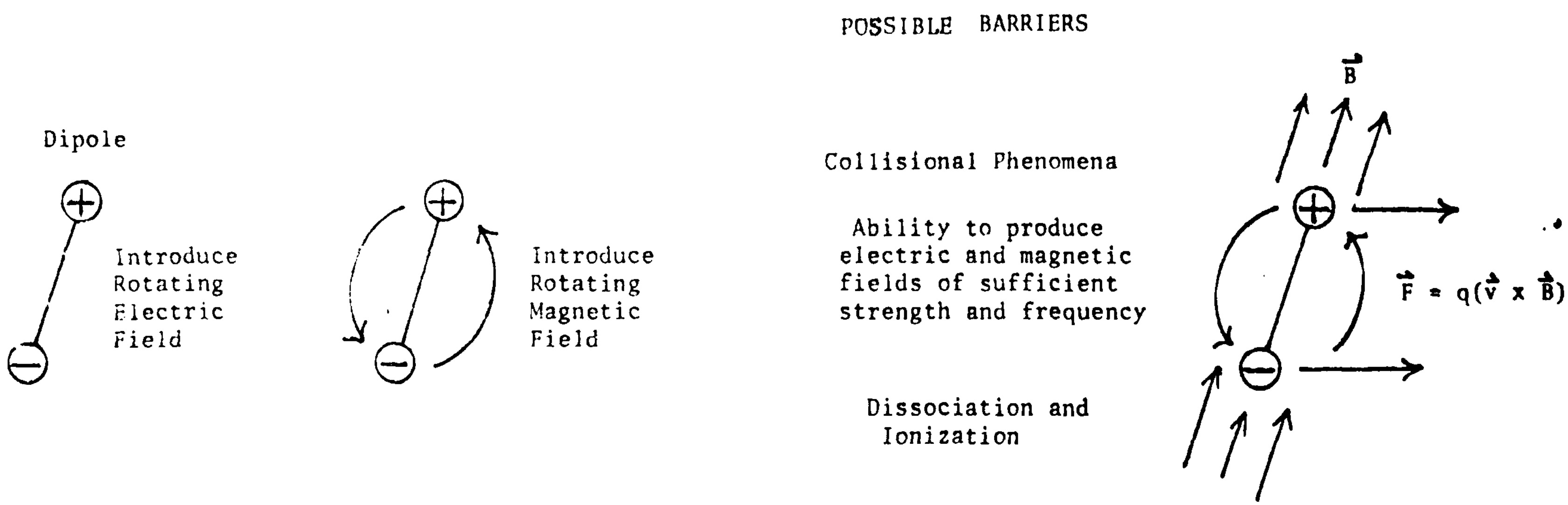

FIGURE 1. Operation and physical problems of ncnionized propulsion method.

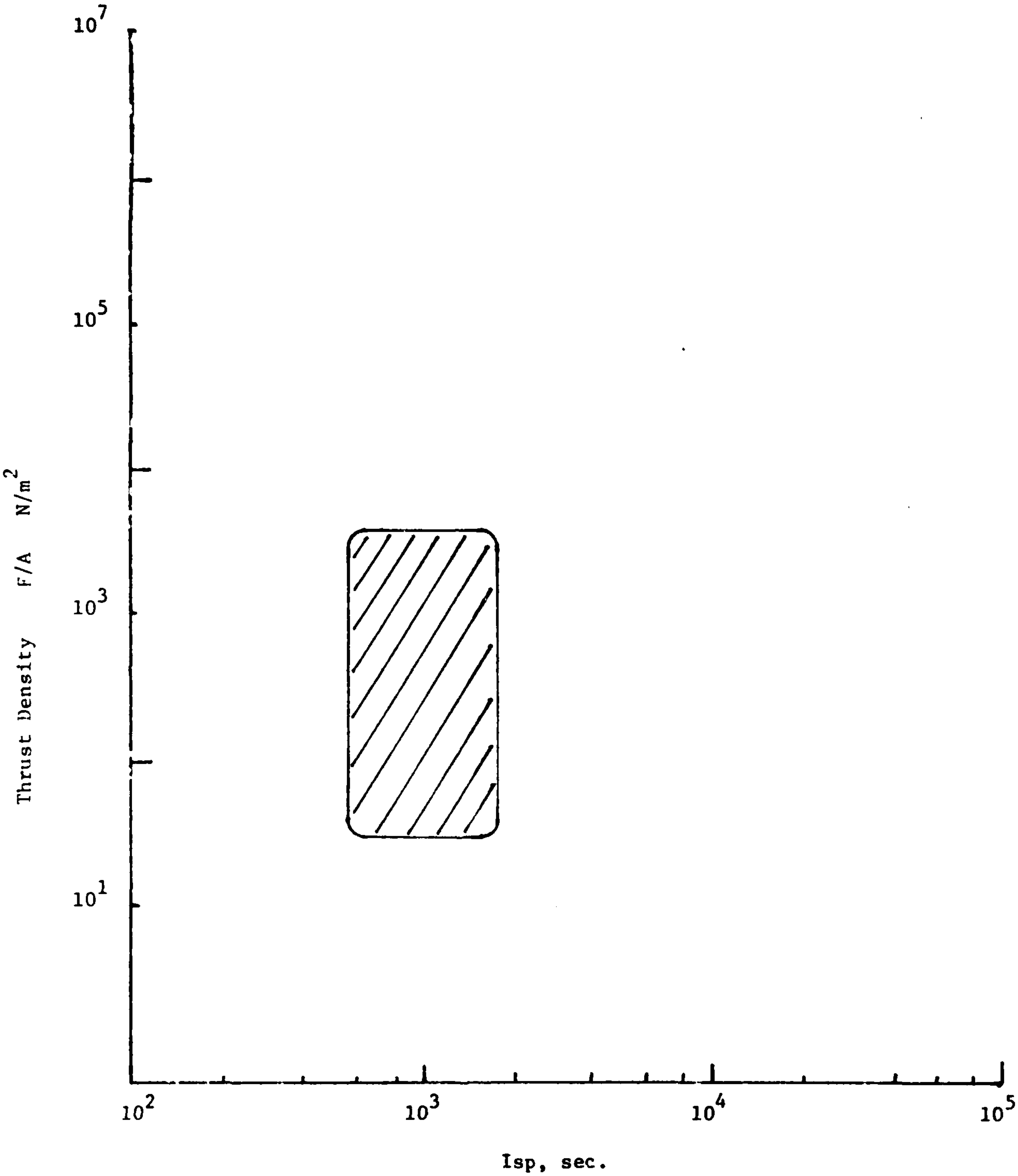

Figure 2. Predicted thrust density versus specific impulse for rotating dipole thruster.

SOLID ROCKET AND SPACE PROPULSION STUDIES

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Purdue University, West Lafayette, Indiana

The sponsored research addresses the following general question of scientific and practical interest: (1) interactions between the steady and nonsteady flowfield in a solid rocket motor and propellant combustion phenomena and (2) the thermal protection of the structure of thrustors powered by radiant energy deposition.

Flowfield/cumbustion interactions have been studied for roughly two decades. However, they have not been clarified to the point where erosive burning in the laminar like flow domains, acoustic erosivity, and velocity coupling are either understood or predictable (linear velocity coupling may not be a physically meaningful way to address that phenomena!) This study will explore the simultaneous use of radiography, magnetic velocimetry, and conventional pressure diagnostics in "real rocket motors" in concert with flow visualization studies. This combination of new and conventional diagnostics is unique because it has potential for direct measurement of the desired interactions in a realistic situation. In radiant energy deposition powered thrustors interactions between the thermal protection system, the internal flow, and the energy deposition process are to be assessed in the light of current understanding to identify the sensitive interactions, and needed research. The unique aspect of this study is that little, if any, trends toward optimal configurations work has been done in this specific area.

Figure 1 illustrates the approach toward flowfield/combustion interaction in solid rocket motors. Three data gathering paths will be explored: flow visualization, radiography, and forced oscillation motor tests. Flow visualization will initially employ the hydraulic analogy; radiography studies will be concerned with accurate burning rate determinations from flash radiographs of rocket motors. By employing appropriate analyses these data inputs will give local mean burning rates directly, (this gives both erosive burning and acoustic aerosivity) pressure coupled response data and information relevent to "velocity coupled driving." The latter is approachable along two lines: the linear analysis of Micci and Caveny (pressure coupled response can be measured independently and simultaneously) and directly by correlation of the nonsteady mechanical energy produced in a segment of the motor (to be measured with two adjacent magnetic velocimeters). Therefore, direct insites into both the adequacies of linear theory and the nature of nonsteady flowfield/combustion interactions will be possible. Theoretical heterogeneous propellant studies are directed at developing a priori burning rate data for pressure coupled response for low and intermediate frequencies. Therefore, the processed data outputs will also clarify the relationships among velocity coupling, acoustic erosivity, and erosive burning and between steady and nonsteady burning.

Figure 2 presents typical results that will occur in this program. The top graph shows rocket motor erosive burning data. The middle graph shows a correlation between experimental and theoretical prediction of the pressure coupled response while the last graph presents the effect of chamber length on impulse decrement (pressure is the parameter) for a radiant energy deposition thrustor.

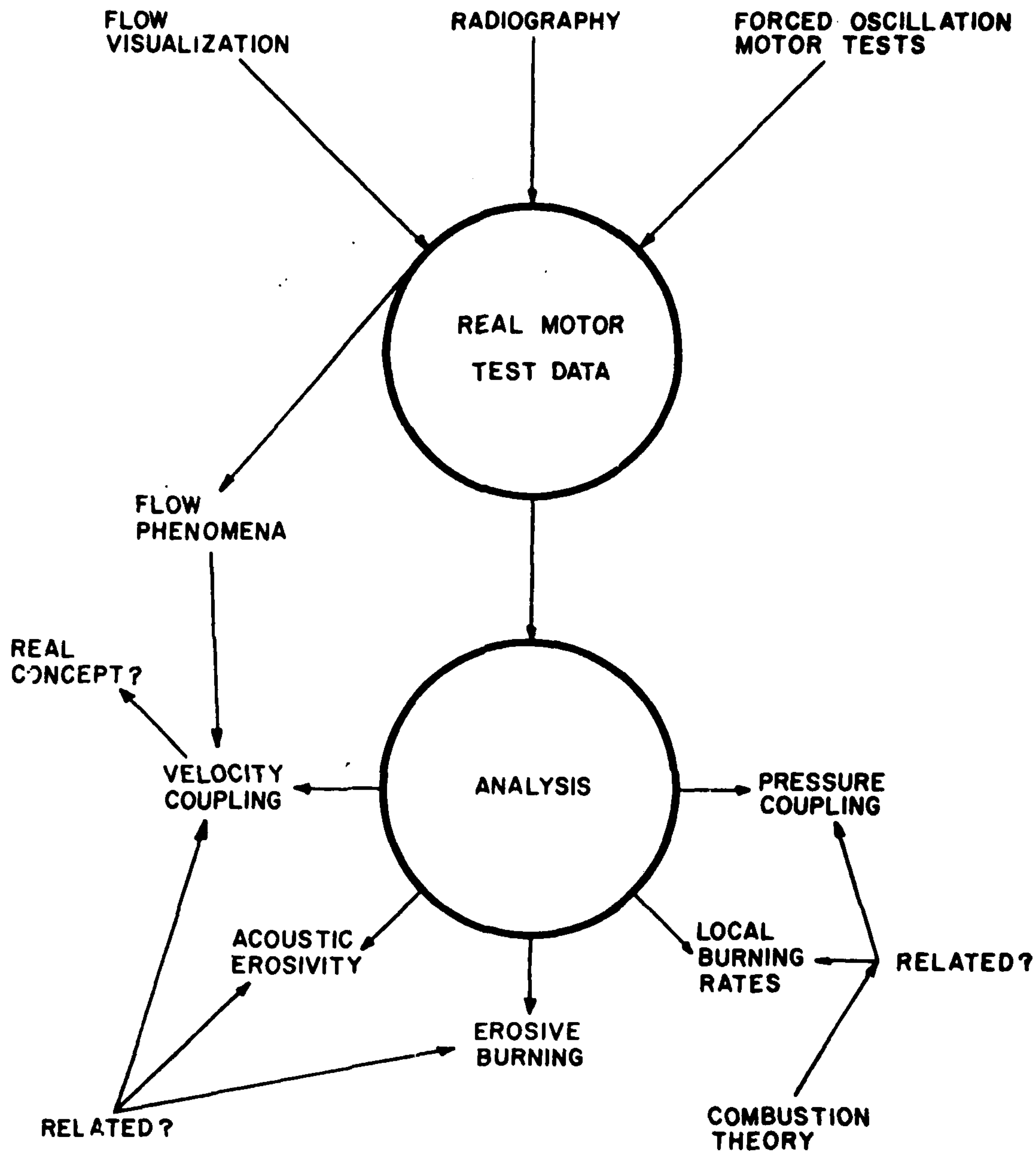
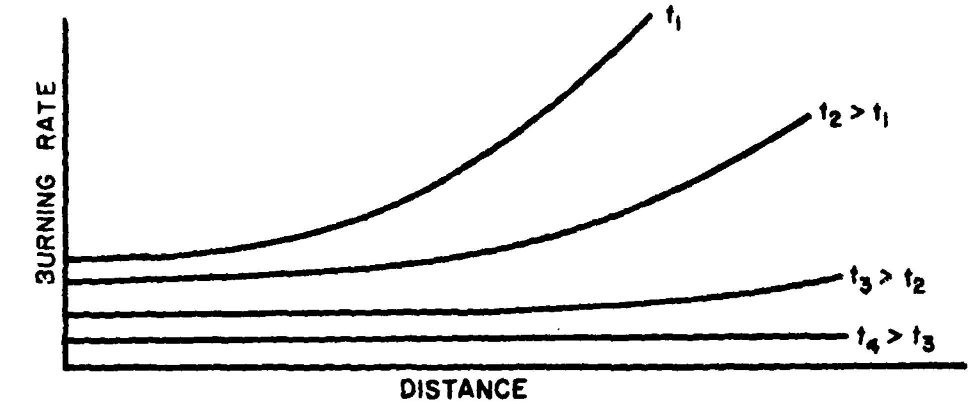
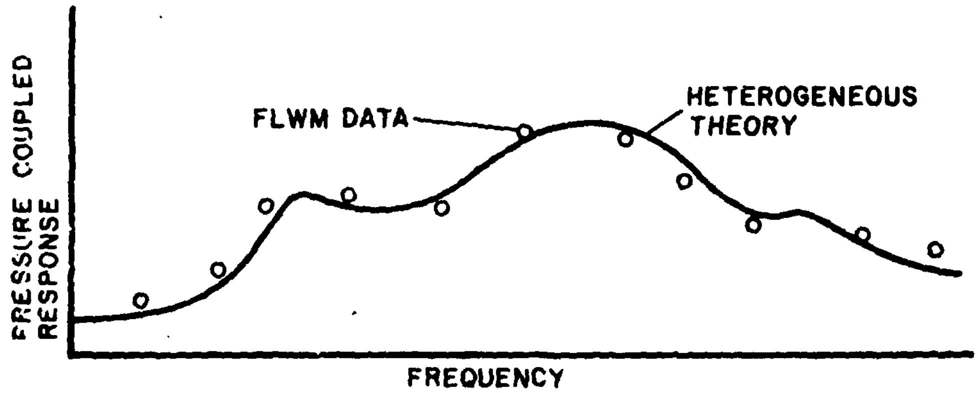


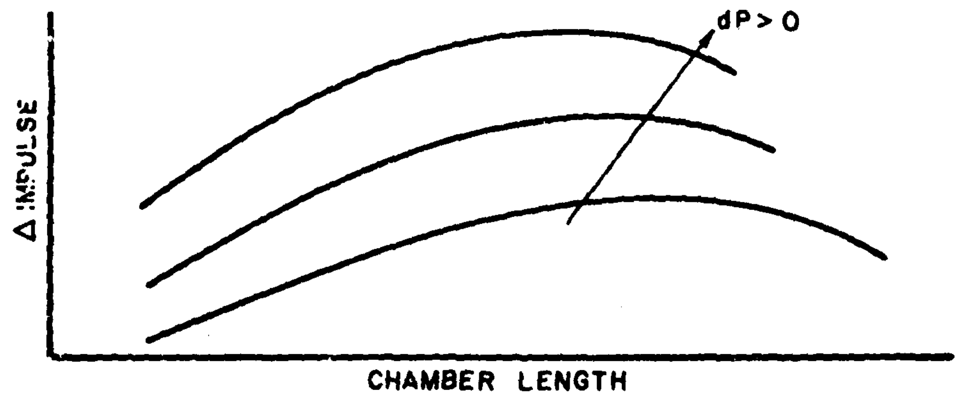
FIGURE 1 APPROACH TO FLOWFIELD/COMBUSTION INTERACTIONS IN A SOLID ROCKET



X-RAY STUDY RESULTS



THEORETICAL COMBUSTION & FLW MOTOR RESULTS



THERMAL PROTECTION STUDY RESULTS

FIGURE 2 RESULTS TO BE OBTAINED

Structural Mechanics Research

Chi T. Liu
Air Force Rocket Propulsion Laboratory
Edwards AFB CA 93523

This research program addresses the fundamental mechanical processes governing fracture, and the statistical nature of crack growth behavior in solid propellants as well as how can they be modeled.

The objective of this program is to gain a better understanding of crack growth behavior in solid propellants. The program consists of three phases over a three year period starting at FY82. The three phases are:

Phase I - (Oct 81 - Sep 82)

- Investigating the statistical nature of crack growth (Fig. 1).
- Determining whether the crack growth rate is controlled by the instantaneous stress intensity factor (Fig. 1).

Phase II - (Oct 82 - Sep 83)

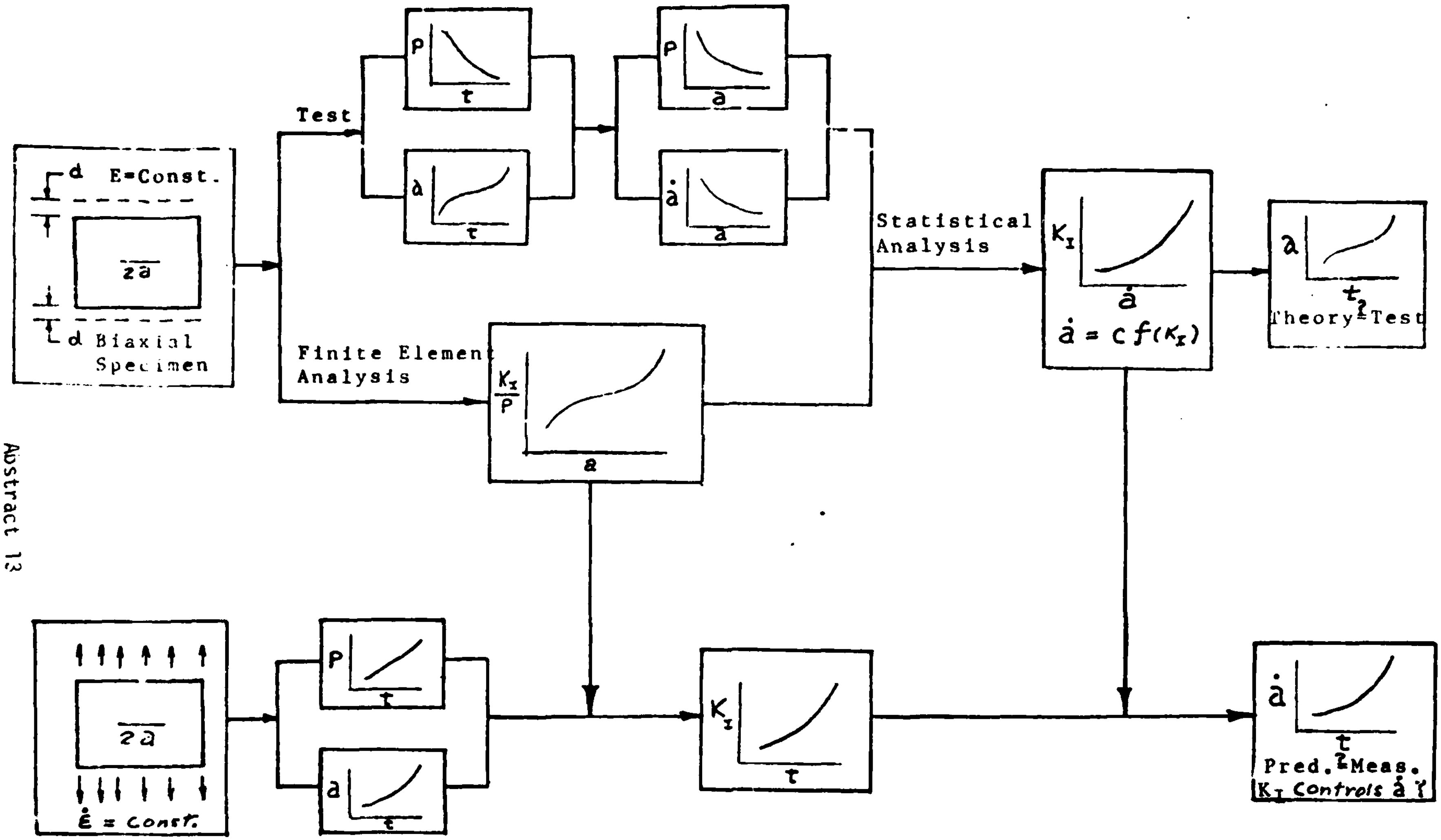
- Determining the role of systematic variation in material property and/or strain in crack growth behavior (Fig. 1).
- Determining the relationship between local strength variation and crack growth behavior based on weakest link theory and probabilistic approach (Fig. 2).

Phase III - (Oct 83 - Sep 84)

- Identifying acoustic emission failure signature and seeking relationship to microscopic failure mechanisms (Fig. 2).
- Determining the relationship between the crack growth rate and the stress intensity factor from acoustic emission data (Fig. 2).

The approach will involve a combination of analytical and experimental studies to develop techniques to investigate crack growth behavior in solid propellants. Finite element methods will be utilized to determine the stress intensity factor and the load on the specimen as a function of crack length. This information will be used in the reduction of experimental data to calculate the stress intensity factor for a given instantaneous crack length and the associated load. Statistical method will be used to treat the test data and a statistical model will be developed. In addition, acoustic emission testing equipment will be used to monitor the crack growth behavior in solid propellants under various loading conditions. The recorded data will be analyzed to investigate the interrelation of acoustic emission and fracture mechanisms in solid propellants.

During the period since Oct 1 81, work has been in progress along the following lines: (1) specimen preparation, (2) finite element analysis, (3) automatic data reduction program and (4) method of crack growth prediction.



a = crack length $\quad$ $\dot{a}$ = crack growth rate $\quad$ P = applied load $\quad$ t = time

K_I = mode I stress intensity factor $\quad$ E = modulus $\quad$ $\dot{\varepsilon}$ = strain rate

d = displacement

N = total acoustic emission counts

FIGURE I SCIENTIFIC APPROACH AND ANTICIPATED RESULT

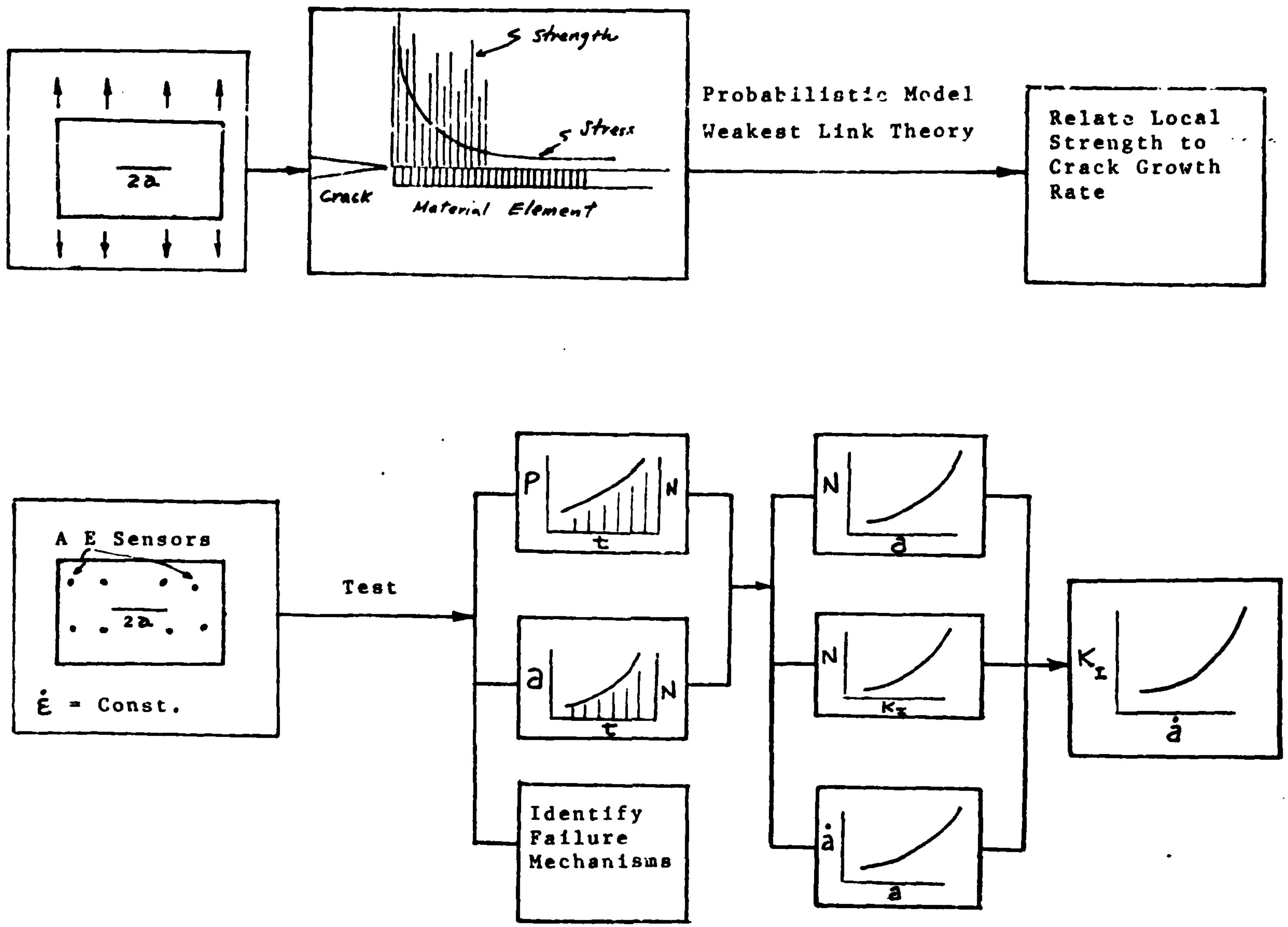


FIGURE 2 SCIENTIFIC APPROACH AND ANTICIPATED RESULT

THERMOMECHANICALLY COUPLED VIBRATIONS IN A CYLINDRICAL GEOMETRY LACKING SYMMETRY; A FINITE ELEMENT SOLUTION PROCEDURE

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The purposes of this project are to develop a general algorithm for the solution of steady state thermomechanically coupled viscoelastic boundary value problems in polar coordinates and to illustrate use of the algorithm on a specific problem.

The materials to be considered are linear viscoelastic solids whose volumetric response is assumed to be elastic. The constitutive relations, however, have a nonlinear thermal term and enough mechanical energy is dissipated into heat that the elevation of temperature cannot be neglected. The equations of thermal and dynamic equilibrium are, therefore, coupled nonlinearly.

The dynamic equations are linear in displacements and their derivatives while the thermal equation is quadratic in the same terms. Given the nature of the constitutive laws, all the field equations contain a nonlinear function of temperature and spatial derivatives of that function. The thermal equation can be linearized in the temperature, however, by using the other equations to express in terms of displacements these thermal nonlinearities. The equations have then been partially linearized and an iterative solution is facilitated. An initial guess for the temperature field is made and the displacement field calculated based upon this guess. Temperatures are then recalculated from the displacements and the process is repeated until convergence is achieved.

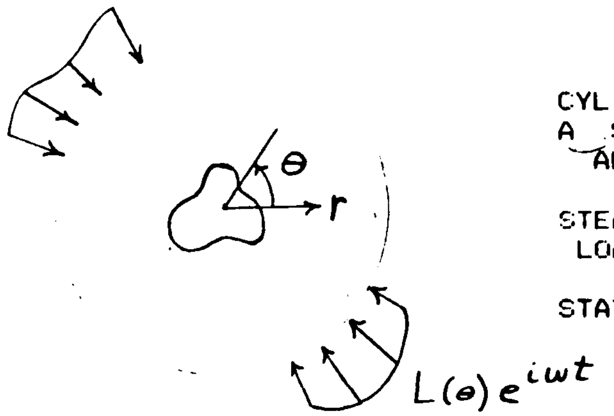
In the iterative algorithm it will be necessary to express the field variables as collections of point values at a finite number of locations and interpolations between those locations. This is best accomplished through use of isoparametric finite elements, which offer geometric flexibility and the necessary continuity of the field variables.

Results of this analysis will be presented in rather general terms. It is to be expected, however, that the solution of any specific boundary value problem will entail numerical difficulties such as troublesome convergence or dependence of the solution upon the mesh configuration. Additionally, solutions of thermomechanically coupled problems are known often to depend discontinuously upon parameters, such as amplitude and frequency, of the forcing functions. For these reasons, one or more specific boundary value problems will be solved as a means of illustrating ways of dealing with these numerical difficulties.

This project is designed to set up a framework for the solution of a class of design problems of interest to AFRPL and to illustrate the practical application of the solution procedure. The results of the research should also provide AFRPL with an enhanced capability numerically to investigate the effect of various constitutive assumptions.

This project is a logical extention of research done by the principal investigator and others on the use of finite differences in solving one-dimensional problems in thermoviscoelasticity and the principal investigator is unaware of any previous extention of that work to two-dimensional problems.

THE PROBLEM AND FEATURES OF ITS MODELING



CYLINDRICAL BODY WITH ASYMMETRIC LOADINGS AND CENTRAL VOID

STEADY-STATE SINUSOIDAL LOADING AND RESPONSE

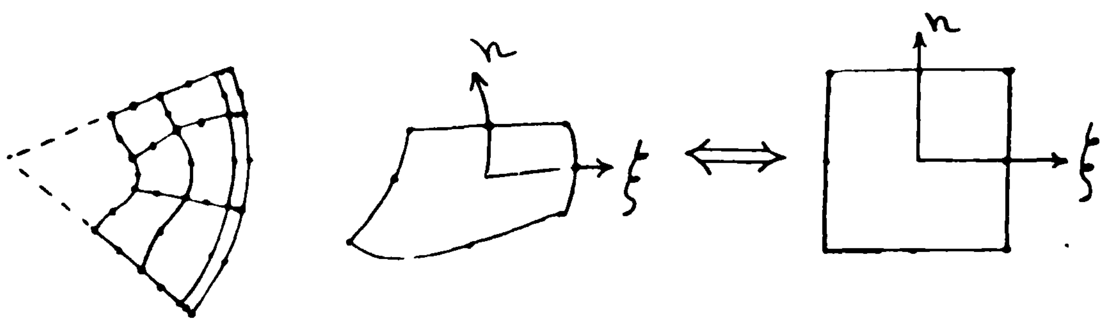
STATE OF PLANE STRAIN

LINEAR THERMOVISCOELASTIC COMPLEX COMPLIANCE

$$(S_1 + iS_2)e^{i\omega t} = G^*(T,\omega)(e_1 + ie_2)e^{i\omega t}$$

ELASTIC BULK MODULUS $\sigma_{VOL} = E_K \, \varepsilon_{VOL}$

DISCRETIZATION OF THE DOMAIN USING ISOPARAMETRIC FINITE ELEMENTS



PARTIALLY LINEARIZED DISCRETIZED FIELD EQUATIONS

$$[K]\,\underset{\sim}{u} = \underset{\sim}{f}(\underset{\sim}{T};\omega) \quad , \quad [D]\,\underset{\sim}{T} = \underset{\sim}{g}(\underset{\sim}{u};\omega)$$

FIGURE 1

PRIMARY GOALS OF THE RESEARCH

1. EQUATIONS OF EQUILIBRIUM IN POLAR COORDINATES

$$-\rho\omega^2 u_m = f_m\left(\sigma^*, \frac{\partial\sigma^*}{\partial r}, \frac{\partial\sigma^*}{\partial\theta}, u_m, \frac{\partial u_m}{\partial r}, \dots, \frac{\partial^2 u_m}{\partial r\partial\theta}\right) \qquad \begin{array}{l} m = 1,2,3,4 \\ n = 1,2,3,4 \end{array}$$

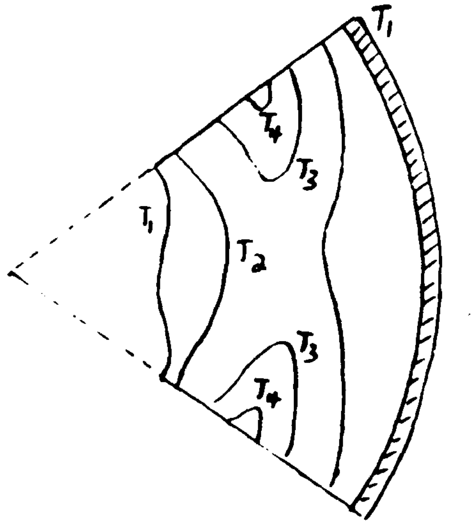
$$-\nabla^2 T = g(\text{SAME ARGUMENTS})$$

2. LINEARIZATION OF THERMAL EQUATION IN TEMPERATURE VARIABLE

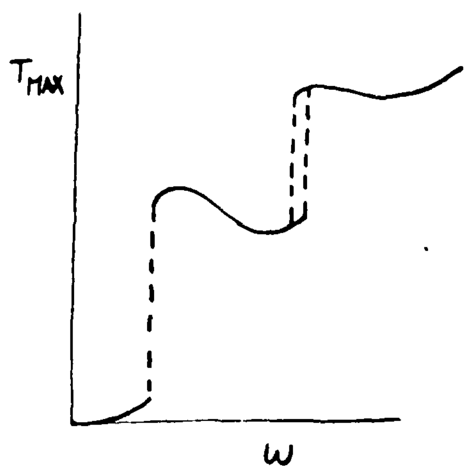
$$-\nabla^2 T = g'\left(u_m, \frac{\partial u_m}{\partial r}, \frac{\partial u_m}{\partial\theta}, \dots, \frac{\partial^2 u_m}{\partial r\partial\theta}\right) \qquad m = 1,2,3,4$$

3. IDENTIFICATION AND JUSTIFICATION OF APPROPRIATE FINITE ELEMENT

4. SOLUTIONS TO BOUNDARY VALUE PROBLEMS FOR SPECIFIC MATERIAL, GEOMETRY AND LOADING



CONTOURS OF FIELD VARIABLES



PARAMETRIC STUDIES

FIGURE 2

COMBUSTION MECHANISMS

D. P. Weaver

Air Force Rocket Propulsion Laboratory
Edwards AFB, CA

An accurate understanding of the details of the combustion processes in solid propellant rocket motors is fundamental to continued successful propellant development and improvements in motor performance. Unfortunately, the motor chamber presents an unacceptably hostile environment for the study of such reaction kinetics. A high pressure window bomb, consisting of a metal cylinder fitted with ports for optical access, has been developed to provide a laboratory scale, high pressure combustion environment. Data on the temperatures, species concentrations, and particle size in this laboratory scale device are essential to assess the validity of such bomb results as applied to motor situations and to provide guidance for continued model development. In the latter area, the more sophisticated calculations which are currently required to accurately model propellant behavior (burn rate, exponents, etc.) cannot be credible without direct comparison with detailed measurements of combustion processes.

Spectroscopic investigation of the combustion of propellants in high pressure combustion bombs will provide new and valuable information in two areas of solid propellant conbustion studies: identification and characterization of intermediate combustion species, and an evaluation of the effectiveness of a window bomb as a model for actual motor conditions. Presently, survey UV and visible emission measurements, coherent anti-Stokes Raman scattering measurements on major species (CO, N_2, H_2), laser-induced fluorescence measurements on trace species (OH), vizualization measurements utilizing conventional high speed photographic and Schlieren techniques are underway as well as standard servo-bomb related measurements (burn rate, composition/inhibitor effects). These measurements will provide highly species specific, spatially and temperally resolved measurements at the high temperatures and pressures characteristic of motor chamber environments for both metallized and nonmetallized propellant samples.

PROGRAM GOALS

*EVALUATE FEASIBILITY/LIMITS OF WINDOW BOMB AS LABORATORY-SCALE MODEL OF ACUTAL SOLID ROCKET MOTOR COMBUSTION

*IDENTIFICATION OF COMBUSTION PRODUCTS OBSERVABLE USING THE COMBUSTION BOMB

*OBTAIN DATA IN SUPPORT OF COMBUSTION MODELS

EXPERIMENTAL APPROACH: DATA OBTAINED

*SERVO-BOMB RELATED MEASUREMENTS:

- -Burn Rate
- -Inhibitor Effects
- -Composition Effects
- -Pressure Effects

*UV-VISIBLE EMISSION SPECTROSCOPY: IDENTIFICATION COMBUSTION PRODUCTS

*IR SPECTROSCOPY: IDENTIFICATION COMBUSTION PRODUCTS

*COHERENT ANTI STOKES RAMAN SCATTERING: MAJOR SPECIES CONCENTRATION AND TEMPERATURE

*LASER FLUORESCENCE: TRACE SPECIES CONCENTRATION AND TEMPERATURE

*PARTICLE SIZING (MIE): PARTICLE SIZE DISTRIBUTION FUNCTION

*SCHLIEREN AND HIGH SPEED PHOTOGRAPHY: VIZUALIZATION

EFFECT OF INHIBITOR ON MEASURED BURN RATE
FOR PROPELLANT (W-5* AT 250 PSI)

INHIBITOR	BURN RATE(mm/sec)	BURN RATE INCREASE (Percentage)
None	1.52	
Fiuorocarbon Greast	1.62	7
R-18 Monomer	1.90	25
Apiezon B016	3.30	117

*73.1% by weight HMX

COMBUSTION MECHANISMS

David H. Campbell
University of Dayton Research Institute
Air Force Rocket Propulsion Laboratory
Edwards AFB, CA

The characterization of combustion processes in rocket engine chambers requires experimental measurement of the temperature and species densities for comparison to computer model predictions and for determination of kinetic rate processes needed as input to the computer codes. Traditional intrusive probe techniques are difficult in the harsh environment of a rocket engine, and so various non-intrusive laser scattering diagnostic techniques have been suggested as more appropriate for measurement of species densities and temperatures in rocket engines. For minor species number densities the Laser Induced Fluorescence (LIF) technique is of particular utility due to its ability to produce detectable time and specially resolved signals from low mole fraction intermediate species important in the combustion chemistry. Attention has been directed especially to the hydroxyl (OH) radical because of its importance in the combustion process and because the wavelength needed to pump the molecule to its first excited electronic state can be obtained easily with existing tunable dye lasers. Unfortunately, fast energy exchange processes redistribute energy among vibrational-rotational (VR) states other than the two laser coupled states during the laser pulse and thus complicate the process of calculating absolute number densities from measured fluorescent intensities. In order to evaluate the effects of these processes a combined computational-experimental effort is being conducted to investigate the detailed temporal behavior of the population distribution in the interval energy states of OH during laser excitation in a combustion environment. Both rotational and vibrational level relaxation effects are being considered, where previous studies have only looked at rotational relaxation effects.

The previous years effort has been devoted to the computational part of the study. The detailed temporal behavior of the distribution of population in the vibrational energy levels of OH in a simulated methane-air flame environment during laser excitation from the zeroth vibrational level in the ground electronic state up to the zeroth or first vibrational level in the first excited electronic state (Figure 1) has been investigated by solving the set of vibrational level rate equations. Included in the model are quenching collisions and vibrational transfer collisions with six flame species. The effects of variation in species mole fractions and laser radiation density on the behavior of OH under laser excitation have been evaluated, as well as the effects of variation in the rate constants for quenching and vibration exchange collisions. For a one atmosphere flame at 2000K, and a laser radiation density of 10^{-8} ergs/cm^3-Hz, a typical result shows a breakdown in the simple two level steady state model on a nanosecond time scale (Figure 2) due to buildup of population in the vibrational "bath" levels (those levels other than the two laser coupled levels) as a result of quenching and vibrational exchange collisions which populate these levels during laser excitation. For a step function laser pulse shape, at steady state the deviation of the upper laser excited vibrational level population from the two-level prediction was 13% for 0-0 excitation and 73% for 0-1 excitation, when the relative quenching rates to the manifold of laser vibrational levels follows the relative spontaneous emission rates. For a distribution of quenching rates which is constant for all laser vibrational levels the deviation was about 85% for both 0-0 and 0-1 excitation. These results indicate that for OH number density measurement in flames using LIF, assurances of accuracy better than an order of magnitude will require (a) better information on detailed quenching rates and (b) laboratory measurements which address the time history of the fluorescent signal on a nanosecond time scale.

Addition of rotation relaxation to the computer model and experimental investigation of the time history of population in the rotational and vibrational levels of OH in a laboratory atmospheric flame, and comparison of the computational and experimental results, will be accomplished during the next year. Application of the LIF technique to measurement of both temperature and OH number density in a laboratory scale solid fuel combustion bomb will also be attempted.

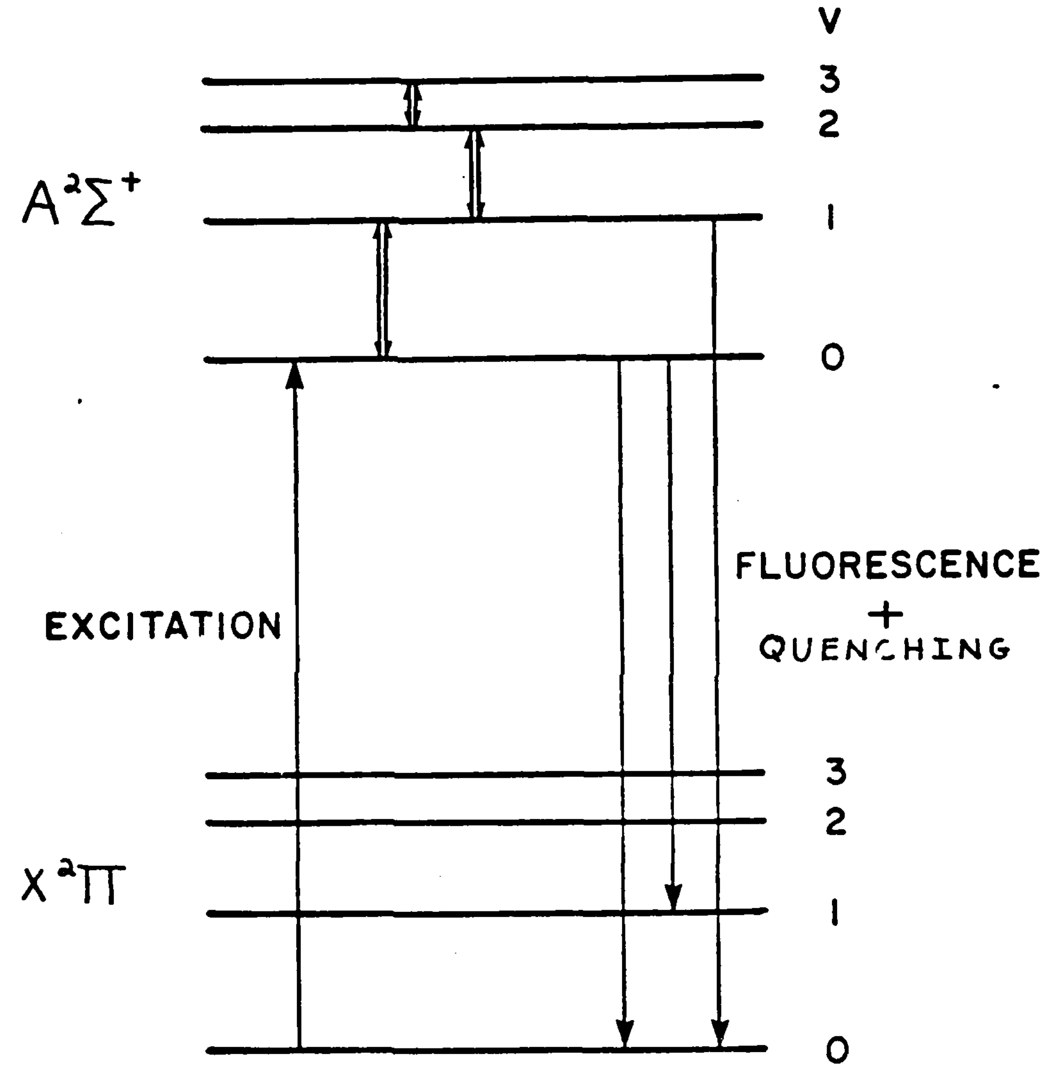


Figure 1. Schematic Diagram of OH Energy Levels Showing Basic Laser-Induced Fluorescence Processes.

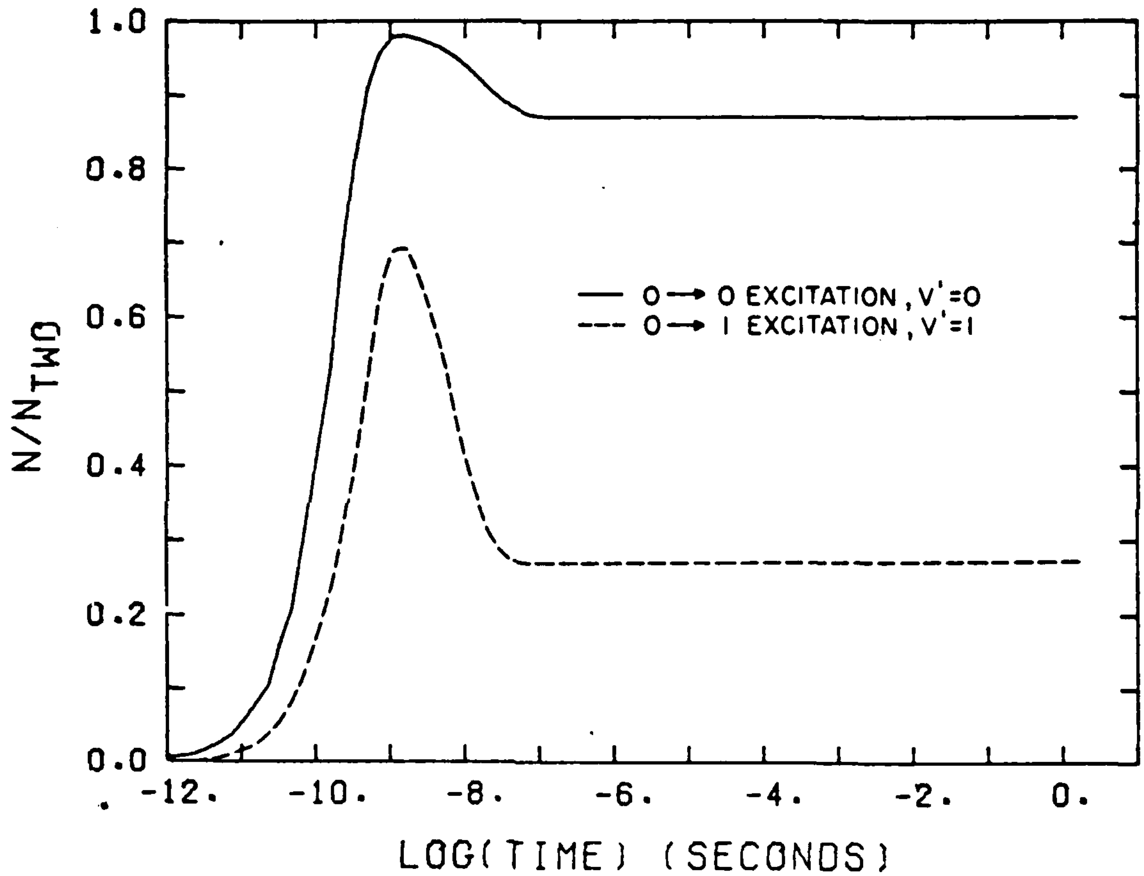


Figure 2. Laser-Excited Upper Level Number Density Time History Normalized by Two-Level Model Prediction for Standard Conditions of 1 atm, 2,000 K for 0→0 and 0→1 Excitation.

MODELING DEFLAGRATION TO SHOCK TO DETONATION TRANSITION (DSDT) IN GRANULAR SOLID PROPELLANTS*

Principal Investigator: Herman Krier
University of Illinois at Urbana-Champaign

The unsteady events associated with the confined burning of granulated solid propellant (due to a damaged solid missile grain) begins with an accelerating deflagration wave supported by convective heat transfer, continues with solid compaction and strong shock formation and in many cases ends with a steady detonation wave, the latter being an obvious propulsion hazard for energetic solid propellants. To analyse the above processes a two phase reactive fluid and solid mechanics model is theorized and in certain cases solved to predict the possible transition to detonation. Figure 1 is a computer solved case where DDT is predicted, showing the pressure history and the deflagration front transition.

Solutions indicating DDT have been published for certain limiting conditions of high surface to volume energetic solids. This effort is depicted as Branch I in Figure 2 and represents one possible scenerio to the potential for DDT. Recent work at Los Alamos National Laboratories with packed beds of granular HMX explosives, separated in a regular pattern by solid interfaces indicates that another scenerio to the detonation transition is possible; this is shown as Branch II in Figure 2. Our efforts are now directed to determine whether one can model this second type of transition process.

The research in progress is summarized as follows: A modification in the conservation-equation transport terms and solid phase equation of state has allowed for initiation of propellant particles under high stress loads by stress heating. In the past, the conservation equations and state equations did not allow for stress heating under the high pressure loads associated with the detonation front.

Basically, the new transport terms in the mass, momentum and energy conservation equation are arrived at by summing all contributions to the systems entropy and systematically eliminating known expressions (i.e., viscous drag conduction) which show up in the inequality. This is achieved by invoking the concept of admissable thermodynamics (in a thermochemical process all terms must individually contribute to the entropy in a positive definite sense) which assures the second law of thermodynamics is satisfied throughout the process.

In our previous model, we imposed the Tait equation of state for the solid phase. This equation assumes the solid phase compression takes place isothermally. The new solid phase equation of state includes a thermal expansion term. The gas phase equation of state remains the same, matching the compressibility factor ($Pv/RT=Z$) at both the CJ state and at ambient conditions.

Coupled with the solid stress equation through a free energy evaluation of the compressible solid is a new expression for the solid phase internal energy. It is now dependent on both temperature and stress whereas in our previous work it was only temperature dependent.

To analyse the DSDT processes one must therefore have the following additional information: (a) the solid phase shock Hugoniot which specifies a density-dependent bulk-modulus; (b) minimum initiation energy due to compressive heating; (c) fracture-mechanics associated with severe shape deformation, and (d) the relaxation constant to specify the pore collapse of the highly stressed granular matrix.

*Work supported by AFOSR under grant No. 81-0145.

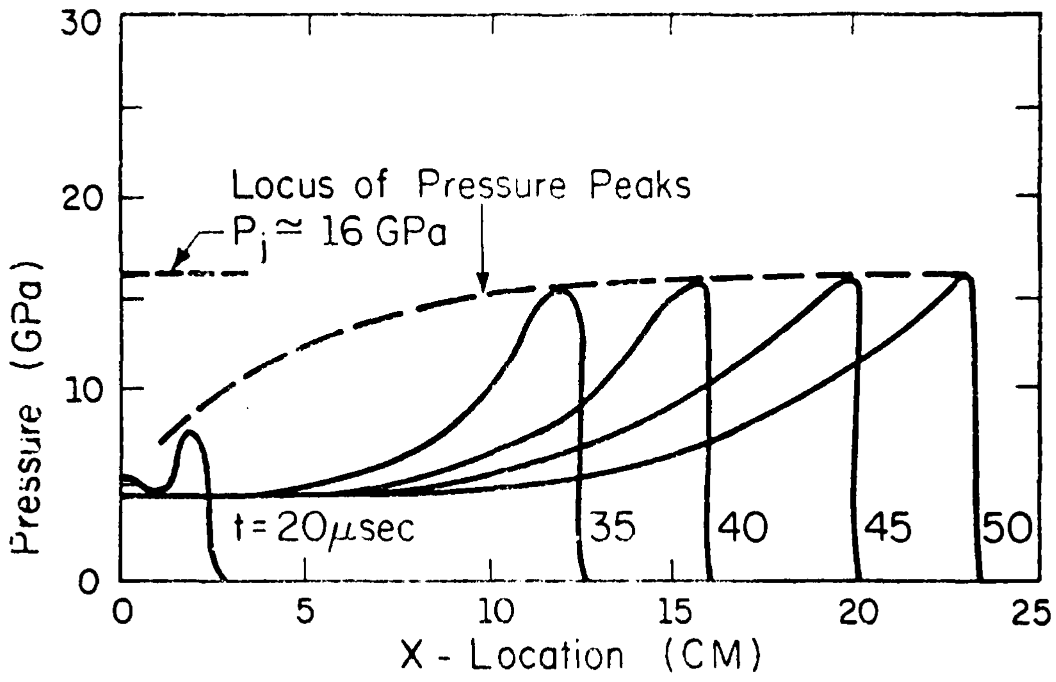


Figure 1a. Pressure History During Accelerating Deflagration in a Packed Bed Leading to a Detonation Transition (n = 1.0).

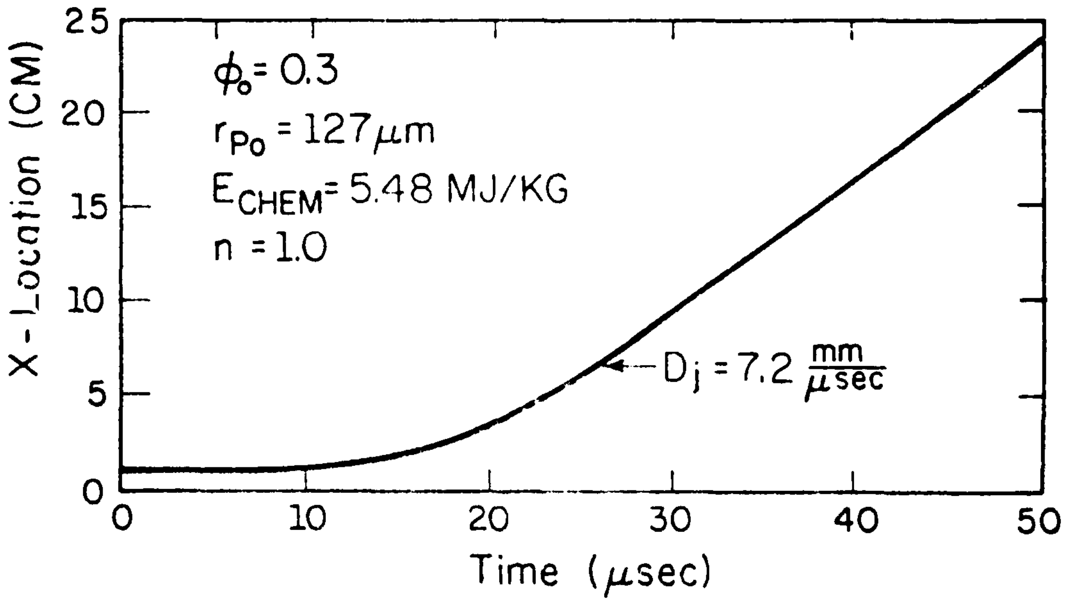
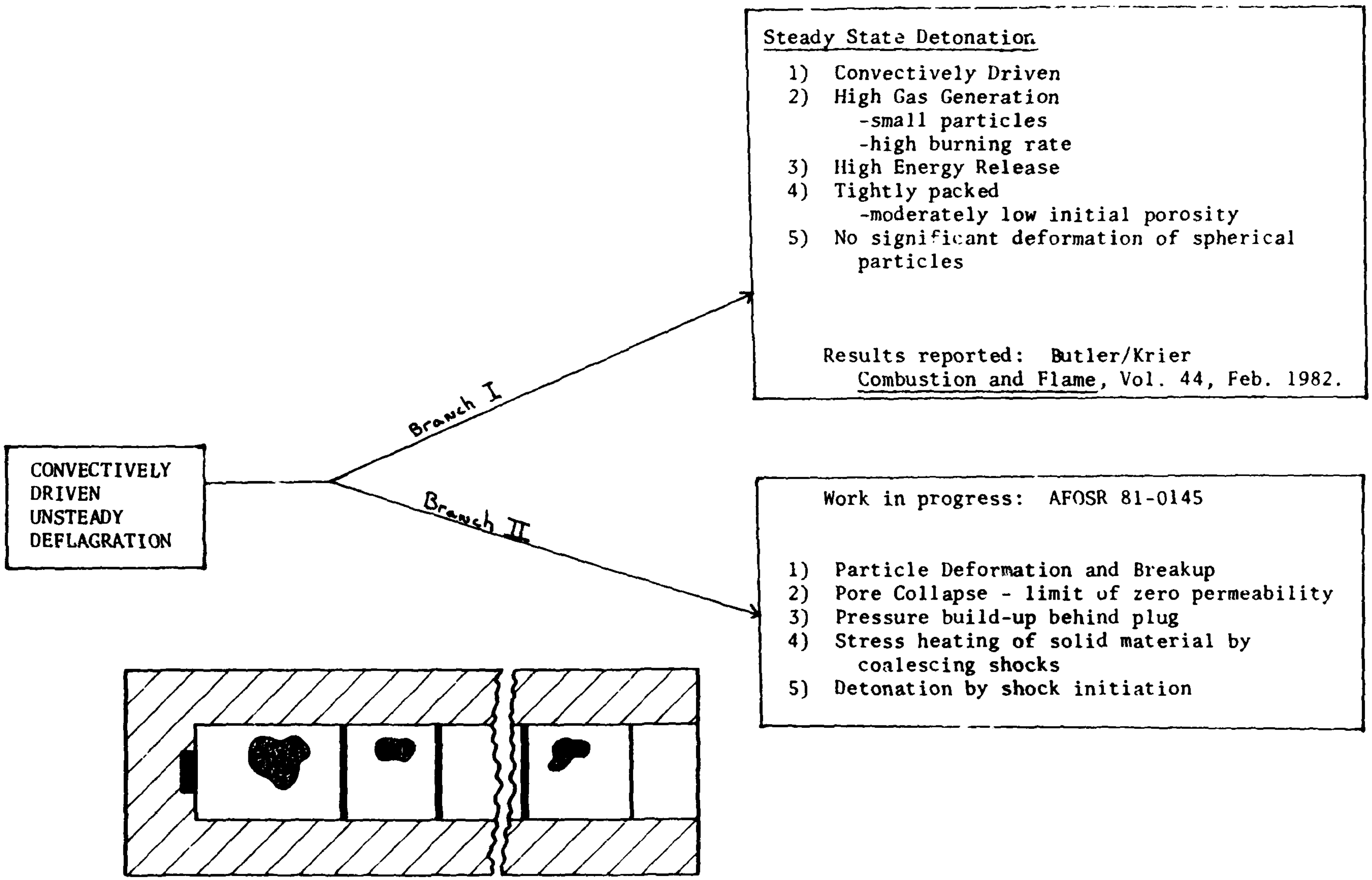


Figure 1b. Ignition Front Locus with Detonation Transition (n = 1.0)

Figure 2: Two Possible Mechanisms for Detonation in Porous Explosives (Propellants)

University of Illinois, Urbana-Champaign



NON-STEADY COMBUSTION OF COMPOSITE PROPELLANTS

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Pasadena, California

The main objective of this research program is to develop an understanding of how and why combustion instability is so strongly affected by ammonium perchlorate particle size distribution. The approach adopted is to study the nature and effects of the composite propellant fine structure, or heterogeneity. Both theoretical analysis and experimental tasks are involved.

The theoretical analysis addresses the effects of compositional as well as pressure fluctuations on the pressure-coupled combustion response function. It is presumed that the fine structure creates periodicities in the propellant formulation which come into play during burning, and which contribute to the driving of pressure oscillations occurring at the same frequencies. The experimental work seeks to characterize these periodicities and their manifestations during propellant burning. Three types of experiments are in progress, Fig. 1. First, the inherent periodicities are determined by densitometer analysis of chlorine-return images of propellants, obtained from a scanning electron microscope employing energy dispersive analysis of x-rays. Second, the JPL microwave burner is used to measure dynamic burning rates at constant pressure, and thereby combustion response to the compositional fluctuations. Third, the microwave burner is used to measure response functions under oscillatory pressures. The inherent periodicities are used to obtain heterogeneity distribution functions as well as establish the existence of preferential frequencies and their dimensional sources in the fine structure. Once the heterogeneity distribution is known, the theory can be used to calculate response functions for comparisons with the data. It is also desired to see whether or not preferential frequencies appear consistently in the various experiments.

The theoretical analysis provides an expression for the response function as the sum of pressure and compositional response components, Fig. 2. Parametric computations have been made over a wide latitude of the controlling variables. The key combustion parameters are found to be burning rate, pressure exponent, temperature sensitivity, and a new parameter referred to as the "concentration exponent" (dependence of burn rate on AP concentration in a form analogous to pressure exponent). Size distribution comes into play through its effects upon these parameters, which have been calculated using a suitable combustion model, and upon the nature of the compositional fluctuations, which is yet to be determined. The compositional response is potentially the dominant source of combustion instability driving because of the tremendous range and variability of the concentration exponent as compared to the pressure exponent.

Experiments to-date have shown the existence of significant compositional fluctuations, Fig. 2, and dynamic burning over a broad frequency range, but the relationship to the size distribution is not immediately obvious. Additional work is needed to perfect the methods to improve resolution and reduce background noise. Questions are raised about the importance of particle shapes, packings and mix isotropicity; these are also of interest to aluminum combustion, various combustion anomalies and mechanical properties.

HOW DOES AP SIZE DISTRIBUTION AFFECT COMBUSTION INSTABILITY?

APPROACH

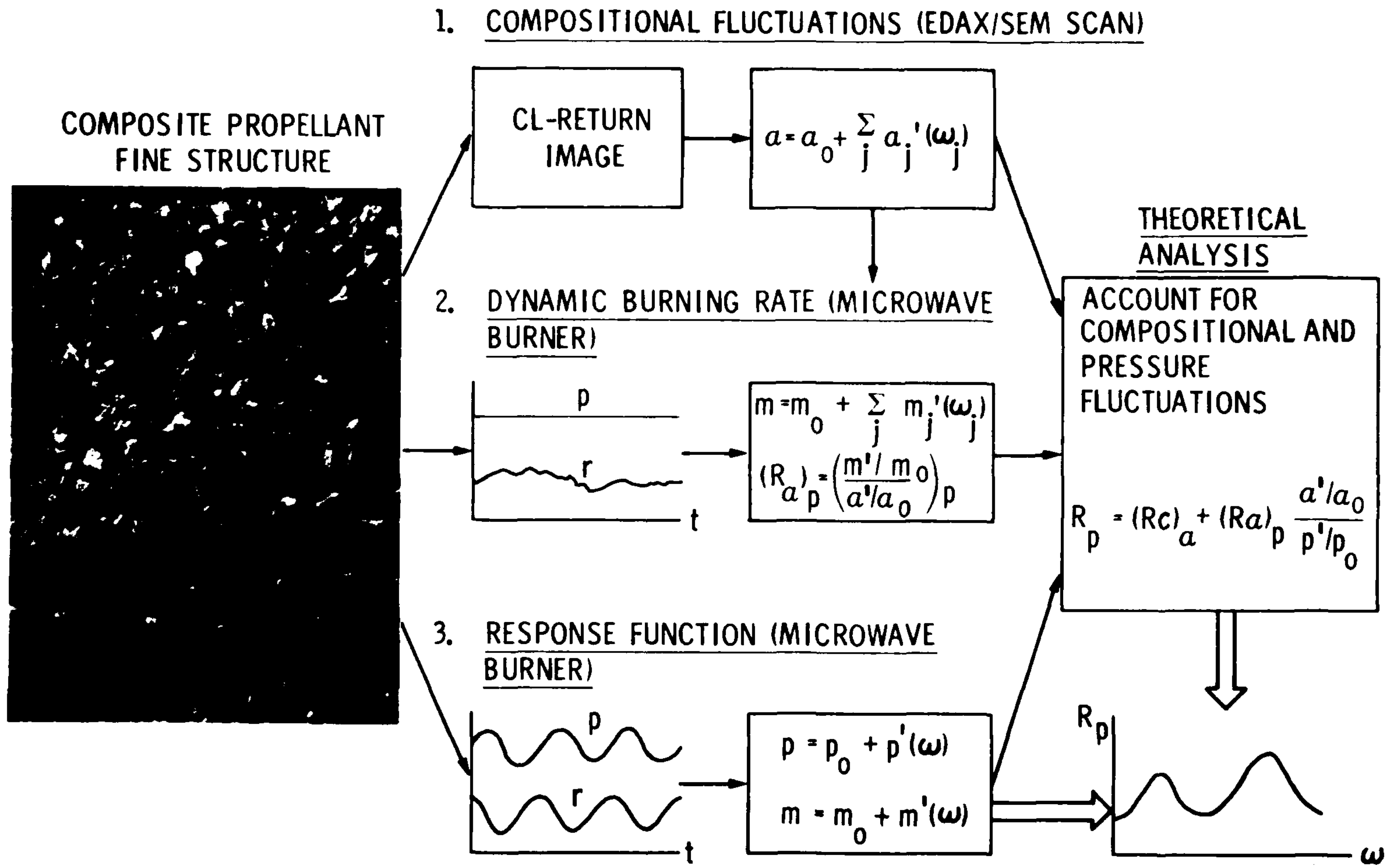


FIGURE 1

PRIMARY ACCOMPLISHMENTS

THEORETICAL ANALYSIS

DENSITY VARIATION WITH % AP

SURFACE TEMPERATURE ABOVE AMBIENT

HETEROGENEITY FORM FUNCTION

$$R_p = \frac{n_p + \left[n_\alpha - K_\rho \sigma_p (T_w - T_0)(1 - \frac{1}{\lambda}) \right] f(D)}{1 - \sigma_p (T_w - T_0)(1 - \frac{1}{\lambda}) + \sigma_T (\lambda - 1)}$$

PRESSURE EXPONENT

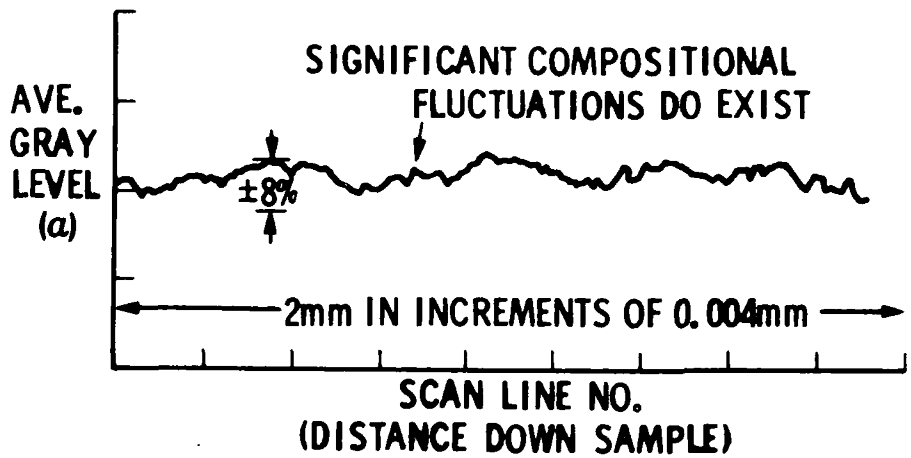
CONCENTRATION EXPONENT

TEMPERATURE SENSITIVITY

RELATED TO σ_P

COMPLEX QUANTITY, FUNCTION OF BURN RATE AND FREQUENCY

EDAX/SEM SCAN ANALYSIS, A-13 PROPELLANT



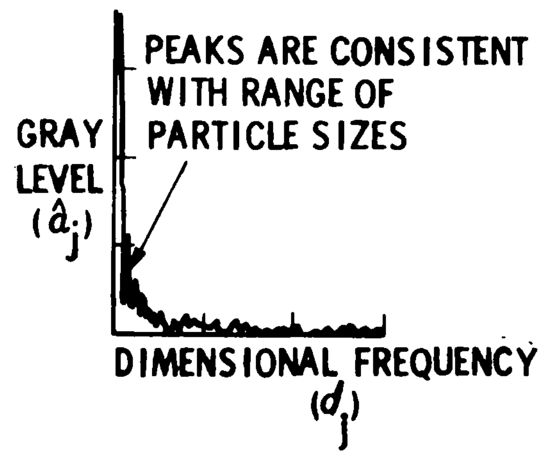


FIGURE 2

AFRPL Research Interests in Rocket Propulsion

DAVID M. MANN
Air Force Rocket Propulsion Laboratory
Edwards Air Force Base, California

Rocket propulsion research strives to provide a basis of information for the solution of existing problems and for step function or revolutionary improvements in all aspects of system performance. The general categories of research and their concerns are:

Propellant Ingredients: Continuing progress in propellant technology requires additional basic understanding of propellants and their constituents as well as the development of new materials with improved capabilities, i.e. higher performance, better mechanical properties, longer life, lower cost, etc.

Solid Propellant Mechanics: The ability to predict the service life of a solid propellant requires the capability to calculate internal stresses and the mechanisms and microscopic processes which lead to large scale failure.

Combustion: Improved rocket performance rests on a better understanding of the combustion processes of gaseous, liquid and solid propellants. It is particularly important to understand the mechanisms controlling both transient and steady state combustion behavior.

Exhaust Plumes: Primary requirements for improved plume characterization are a better understanding of supersonic, turbulent reacting flows and the effects of high particulate loadings on both the gas dynamics and radiative transport in such flows.

Cases, Nozzles and Structures: Improved understanding of the thermal, mechanical and environmental properties of composite materials is needed in order to fully exploit the capabilities of these new materials. Trends towards higher operating pressures and temperatures are seriously pressing materials capabilities.

Advanced Propulsion Concepts: Several non-chemical propulsion concepts offer the potential for very high performance propulsion. These and other concepts need to be studied to overcome the barriers currently impending their use as prime or secondary propulsion systems.

Details will be provided in the above areas and AFRPL points-of-contact identified.

EVALUATION AND COMPILATION OF THE THERMODYNAMIC PROPERTIES OF HIGH TEMPERATURE SPECIES

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The Dow Chemical Company
Physicochemical Studies
Midland, Michigan 48640

The JANAF Thermochemical Tables are a set of continually updated self-consistent thermodynamic data currently available in a well-established format which can be quickly and easily used. These tables result from reviewing all literature sources, evaluating the accuracy of the experimental data/-theoretical calculations, calculating temperature-dependent thermodynamic functions, and publishing thermochemical tables for use in the Air Force community. Considerable effort is directed to discussing both the uncertainties in the data and the experimental data necessary to reduce this uncertainty.

The selection of species to be studied depends on current and future Air Force interests. In generating the obvious products of this project, there are three main concerns currently of interest. First and foremost, the upcoming publication of a "third edition" is necessitating an updating of all the elemental reference states. Second, the aluminum- and boron-containing species are being refined for inclusion in the third edition. The emphasis is not only to provide current reliable tables in this area but also to highlight and prioritize the missing/weak experimental data. Third, cooperative ventures are playing an important role in reducing duplicative efforts.

JANAF THERMOCHEMICAL TABLES

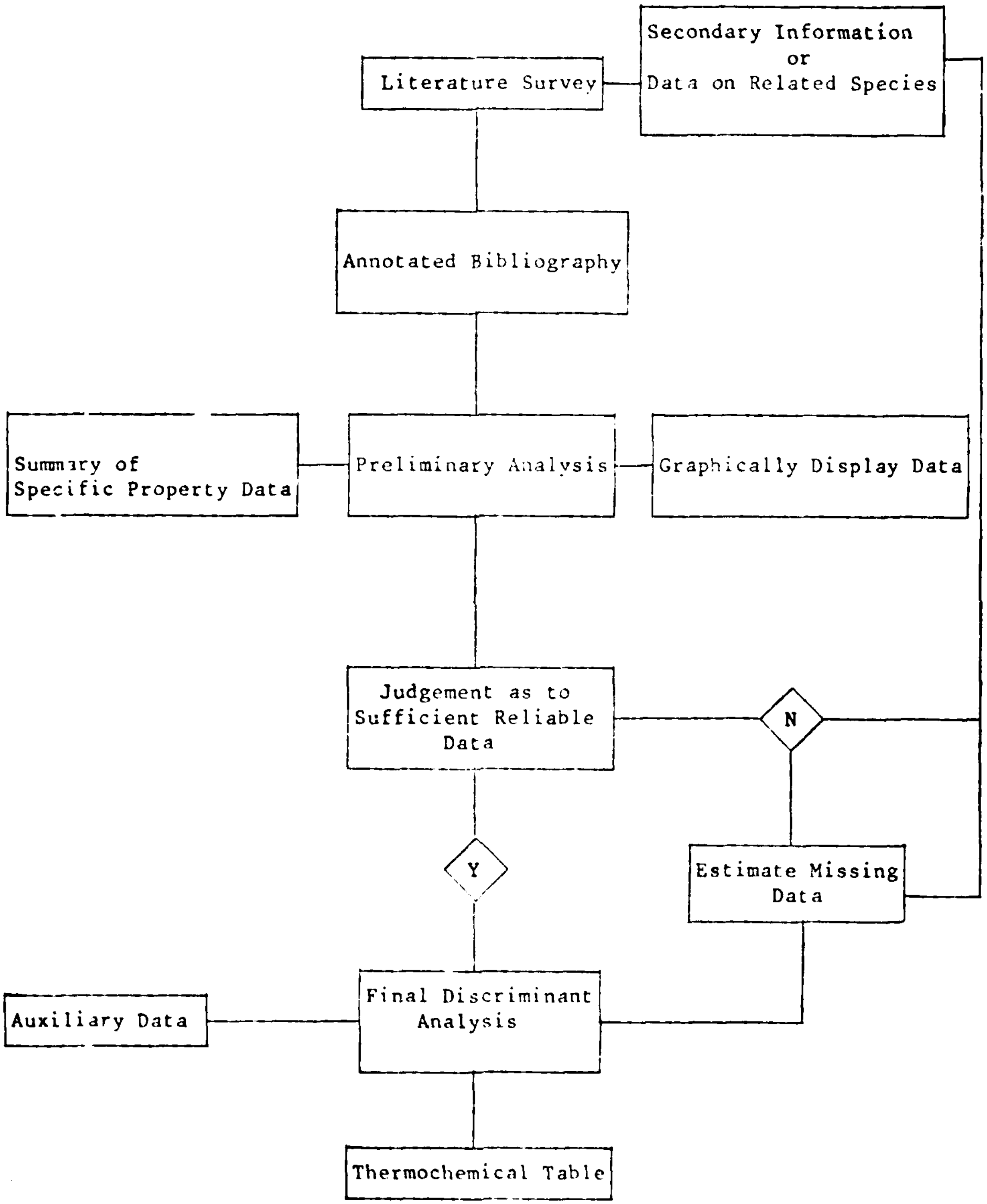

FIGURE 1

JANAF THERMOCHEMICAL TABLES

DOW CHEMICAL U.S.A.
Physiochemical Studies
1707 Building
Midland, Michigan 48640

Telephone: (517) 636-4160

Date Established	1959.
Sponsoring Organizations	U.S. Air Force, Office of Scientific Research (AFOSR). Dr. Leonard H. Caveny U.S. Department of Energy, PETC/Combustion Division. Francis E. Spencer, Jr. Technical Project Officer.
Heat of This Unit	Dr. Malcolm W. Chase, Project Director.
Contributors	Patricia A. Andreozzi, Carol A. Davies, Joseph R. Downey, Jr. Richard A. McDonald, Alan N. Syverud, Edward A. Valenzuela, and Robert L. Vance
Description of System or Service	JOINT ARMY-NAVY-AIR FORCE THERMOCHEMICAL TABLES (JANAF) are compilations of thermochemical data for species of interest at high temperatures and of thermodynamic properties as a function of temperature. JANAF THERMOCHEMICAL TABLES are obtained by a careful search, critical evaluation, and selection of the literature or by the estimation of certain data, and published with a complete discussion of the data treatment and selection as well as the inclusion of all pertinent references.
Scope of Subject Coverage	Heat capacity, enthalpy, entropy, free energy functions, heats, and free energies of formation for compounds of the elements H, D, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Ti, V, Cr, Fe, Co, Ni, Cu, Zn, Br, Kr, Sr, Zr, Nb, Mo, I, Xe, Cs, Ba, Hf, Ta, W, Hg, and Pb.
Input Sources	Published and unpublished chemical literature.
Holdings of Recorded Data	Data base consists of the tables and the references used to compile them.
Serial Publications	Supplements to JANAF THERMOCHEMICAL TABLES (quarterly) - in loose-leaf form; available to recipients approved by AFOSR or DOE contract monitor.
Non-serial Publications	JANAF THERMOCHEMICAL TABLES, Supplements 1-17, 1959-1965, published as PB 168 370; supplements 18-29, 1966-1968, published as PB 168 370-1, PB 168 370-2, PB 168 370-3. These publications are obsolete. Supplements 1-33, 1971, are contained in "JANAF Thermochemical Tables, Second Edition, NSRDS-NBS-37, Catalog number C13.48:37," available through U.S. Government Printing Office, Washington, D.C. 20402. NSRDS-NBS-37, supercedes the four PB publications. Supplements 34-37, published in J. Phy. Chem Ref. Data 3(2), 311-480 (1974); Supplements 38-41 published in J. Phys. Chem. Ref. Data, Vol. 4(1), 1-175(1975); Supplements 42-45, published in J. Phys. Chem. Ref. Data 7(3), 793-940 (1978). Supplement 46-52 to be published in J. Phys. Chem. Ref. Data.
Magnetic Tape Services	Supplements 1-current, with numerical values only (no writeup or references) are available on tape with individual supplements extra.
Computer and Information Processing Equipment	Tables utilize IBM 3033 computer with PL/1, COBOL, FORTRAN IV, and BASIC as program languages.
User Equipment Requirements	Magnetic tapes are in IBM EBCDIC, 800/1600/6250 bpi, 9 track.

CRITICAL EVALUATION OF HIGH TEMPERATURE CHEMICAL KINETIC DATA

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and

Lewis H. Gevantman
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Gaithersburg, Md.

The rapid growth in chemical kinetic data, and simultaneously in the number of nonspecialists who require such data in DOD-related work, has created a need for a reliable, easy-to-use compilation of evaluated rate data and recommended rate coefficients. To answer this need, a program for the evaluation of kinetic data and for the preparation of consistently formatted data sheets patterned after the JANAF Thermochemmical Tables was undertaken in 1978 with the joint support of the Air Force Office of Scientific Research and the National Bureau of Standards. The front of one such data sheet is shown in Fig. 1.

The first task of this program was to examine other approaches to data evaluation and compilation and to develop a compact format of broad utility. Succeeding tasks were to develop the methods for using theory to assess the reasonableness of the experimental measurements and to extrapolate them to higher temperatures. High-temperature data are of special interest to the Air Force, and this is the first data-evaluation program that routinely extrapolates rate coefficients for bimolecular reactions using methods more sophisticated than the familiar Arrhenius expression. Theory is also used to predict rate coefficients for important reactions for which there are no experimental data. The steps involved in preparing a data sheet are shown in Fig. 2. Periodic revisions are made as new experimental data or better theoretical methods become available.

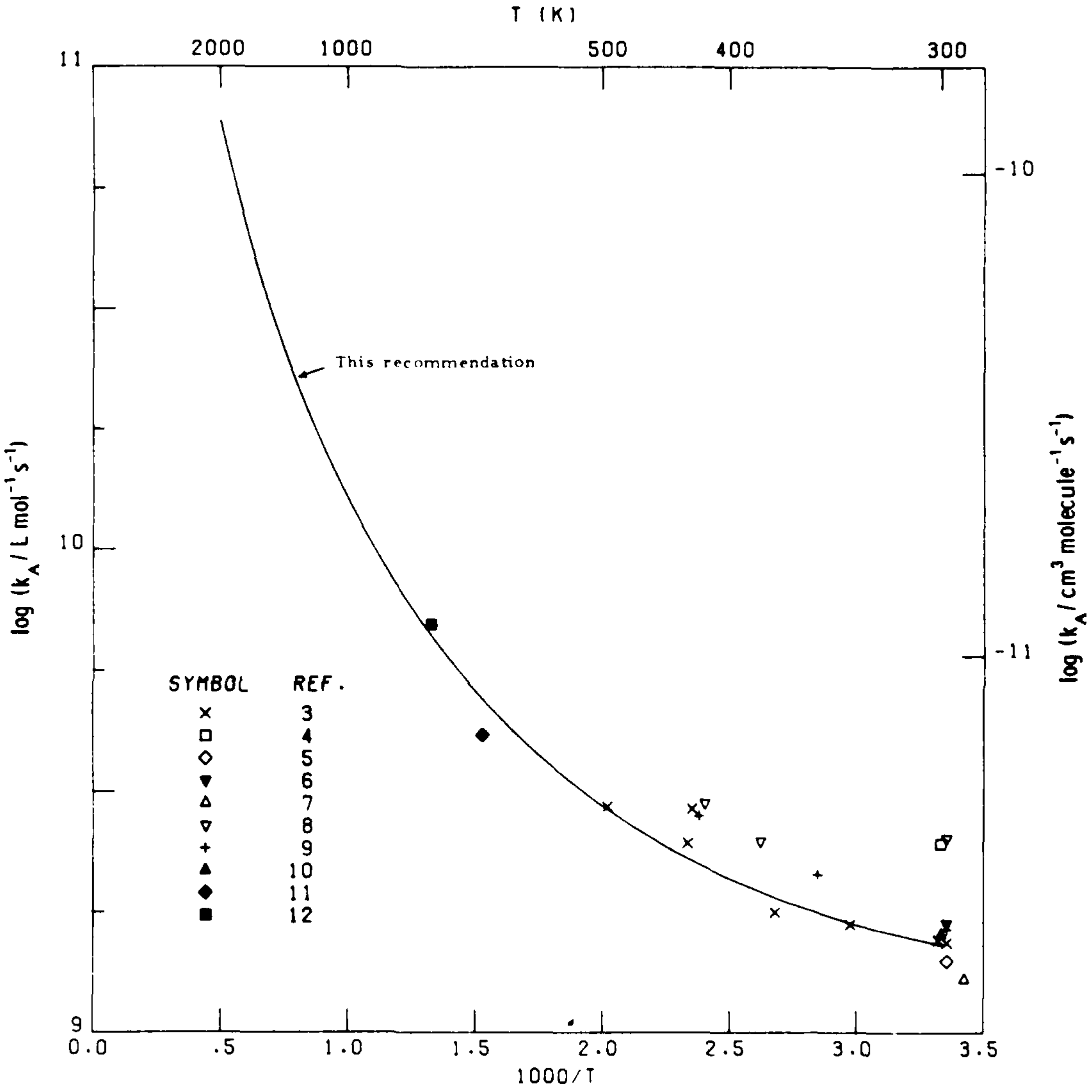
To date 34 sheets have been prepared for reactions of interest of various Air Force programs. These include six reactions important in hydrogen-oxygen combustion ($H + O_2$, $O + H_2$, $OH + H_2$, $OH + OH$, $H + H + M$ [2 sheets]); six in hydrogen halide chemical lasers ($H/D + F_2$, $F + H_2/D_2$, $H + Cl_2$, $Cl + H_2$); 15 in hydrocarbon oxidation (OH + methane, ethane, propane, butane, isobutane, cyclobutane, cyclopentane, pentane, isopentane, neopentane, cyclohexane, 2,3-dimethylbutane, 2,2,3-trimethylbutane, octane, neooctane), five in aluminum or boron propellant systems ($Al + O_2$, $AlO + H_2$, $AlO + OH$, $AlOH + OH$, $B + O_2$); and two in the oxygen-iodine chemical laser ($O_2(^1\Delta) + O_2(^1\Delta)$ and $O_2(^1\Delta) + I(^2P_{1/2})$). Our choice was made partly to test the suitability of the approach for reactions ranging from those for which experimental data are plentiful to those for which no data are available.

The preparation of the series of data sheets for OH + alkane reactions has been accompanied by theoretical efforts to develop a method for using transition state theory to extrapolate experimental data to higher temperatures. The theoretical approach for reactions with such large molecules is quite different from what can be done with simple reactions, such as $F + H_2$, for which reliable a priori potential energy surfaces are available.

$$OH + n\text{-}C_4H_{10} \xrightarrow{A} C_4H_9 + H_2O$$

$OH + n\text{-}C_4H_{10} \xrightarrow{1} n\text{-}C_4H_9 + H_2O$ $\Delta H^o_{298} = -89 \pm 4$ kJ mol^{-1} (-21.3 kcal mol^{-1}) $\Delta S^o_{298} = 16 \pm 4$ J mol^{-1} K^{-1} (4.0 cal $mol^{-1}K^{-1}$)

$OH + n\text{-}C_4H_{10} \xrightarrow{2} s\text{-}C_4H_9 + H_2O$ $\Delta H^o_{298} = -104 \pm 4$ kJ mol^{-1} (-24.8 kcal mol^{-1}) $\Delta S^o_{298} = 20 \pm 4$ J mol^{-1} K^{-1} (4.7 cal $mol^{-1}K^{-1}$)



RECOMMENDED RATE COEFFICIENTS

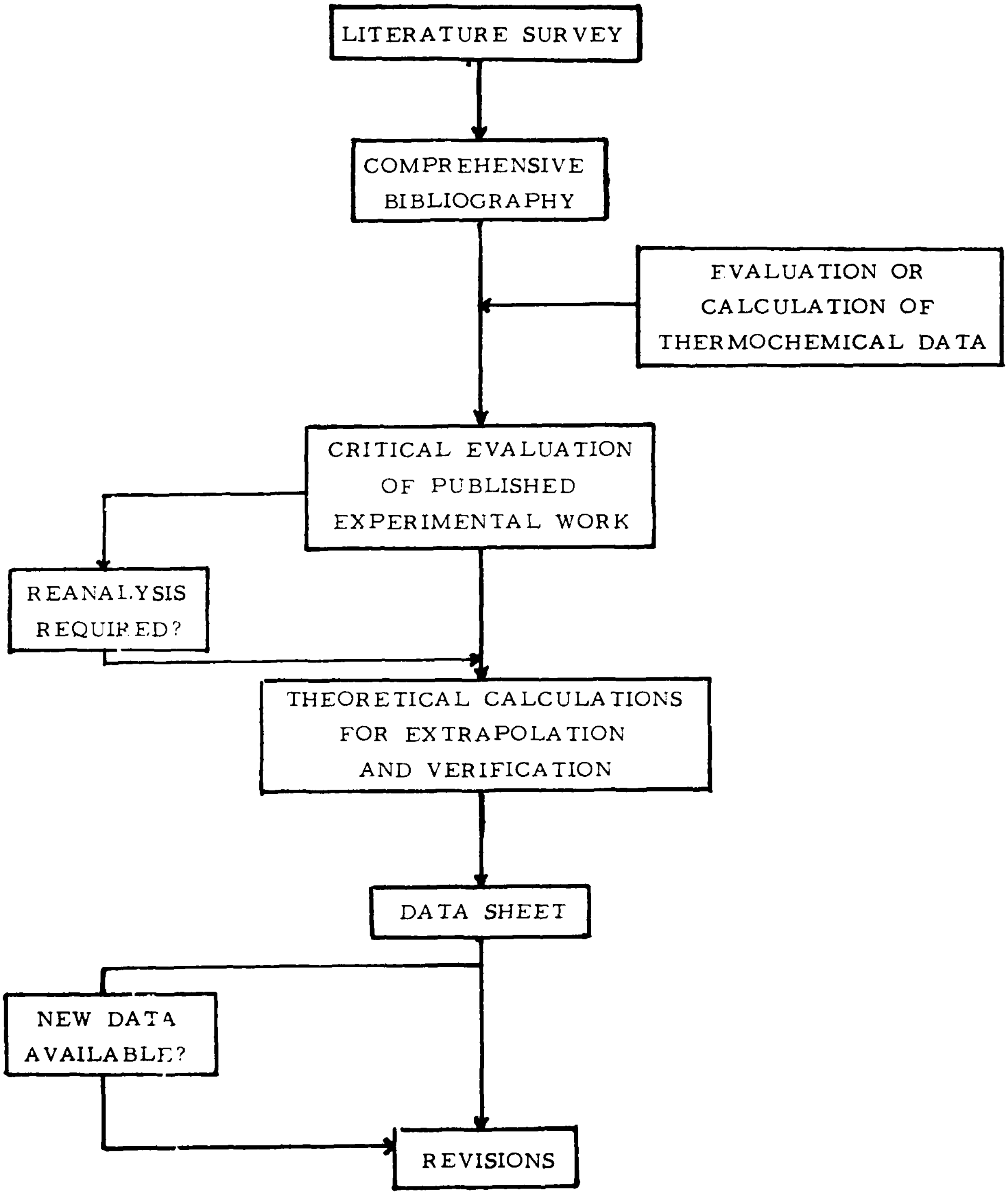
k	k(T)	Range	k(298)	Units
k_A	$6.2 \times 10^4\ T^{1.8} \exp(-55/T)$	300-2000 K	1.5×10^9	L $mol^{-1}s^{-1}$
	$1.0 \times 10^{-16}\ T^{1.8} \exp(-55/T)$		2.5×10^{-12}	cm^3 $molecule^{-1}s^{-1}$
k_1/k_2	$1.1 \exp(-615/T)$	300-2000 K	0.14	---

Uncertainty in log k_A: ±0.1 at 300 K, increasing to ±0.5 at 2000 K. Uncertainty in log k_1/k_2: ±0.3. Because the reverse reactions are unimportant at any temperature; values for K(T), k_{-1} and k_{-2} are not recommended.

(March 1981)

Figure 2

CHEMICAL KINETICS DATA SHEETS



CARBON-CARBON PROCESSING VARIABLES INVESTIGATION

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AIR FORCE ROCKET PROPULSION LABORATORY

AFRPL/MKBN EDWARDS AFB CA 93523

The chemistry and physics of carbon-carbon composites is not well understood even though they are being evaluated as nozzle materials in a number of Air Force programs. This lack of understanding includes the surface ablation kinetics of these materials. There is conjecture about the specie (s) principally responsible for recession. However, there is no definitive data available either pertaining to the principle specie (s), or to the kinetics of the heterogeneous reactions with carbon under rocket nozzle conditions. Therefore, the nozzle designer has no firm theoretical basis on which to predict the performance of his nozzle design. He is forced to make predictions based on data from actual motor firings. The nozzle and conditions used in these firings may or may not represent the composite material and operating conditions that the designer has chosen. The objective of this program is to fill this gap in our knowledge of surface reaction kinetics and their relation to carbon-carbon material construction and processing. This is being accomplished by (1) extensive surface characterization of the carbon-carbon materials and (2) by measuring the kinetics of the heterogeneous reactions between carbon-carbon materials and the various species present in the rocket motor exhaust. This will give the designer a firm basis on which to predict the performance of his nozzle.

During this past year, work continued on the build-up of the new ablation system, which will use a heliostat in conjunction with a solar concentrator to heat the carbon sample. On site we now have the solar concentrator, heliostat, and shutter system. The test chamber has been designed and fabricated and has undergone testing at the University of Dayton. While this build-up has progressed, a Materials Characterization Laboratory capable of characterizing the porosity, active surface area (ASA), total surface area, and the microstructure of the carbon-carbon composites has been completed. Studies have been initiated on nozzle constituents as well as slices from commerically produced nozzles.

Initial characterization work has centered on Pitch (USB-32) and PAN (T-300) carbon fibers used in contemporary nozzle construction. Although these fibers have been found to have similar total surface areas, they have been found to have significantly different pore structures and active surface areas. The differences in active surface areas have been found to track differences in recession properties. Due to the slowness of the ASA measurement process and the current need for the data, two additional systems capable of measuring ASA were recently fabricated for routine data collection.

SCIENTIFIC APPROACH

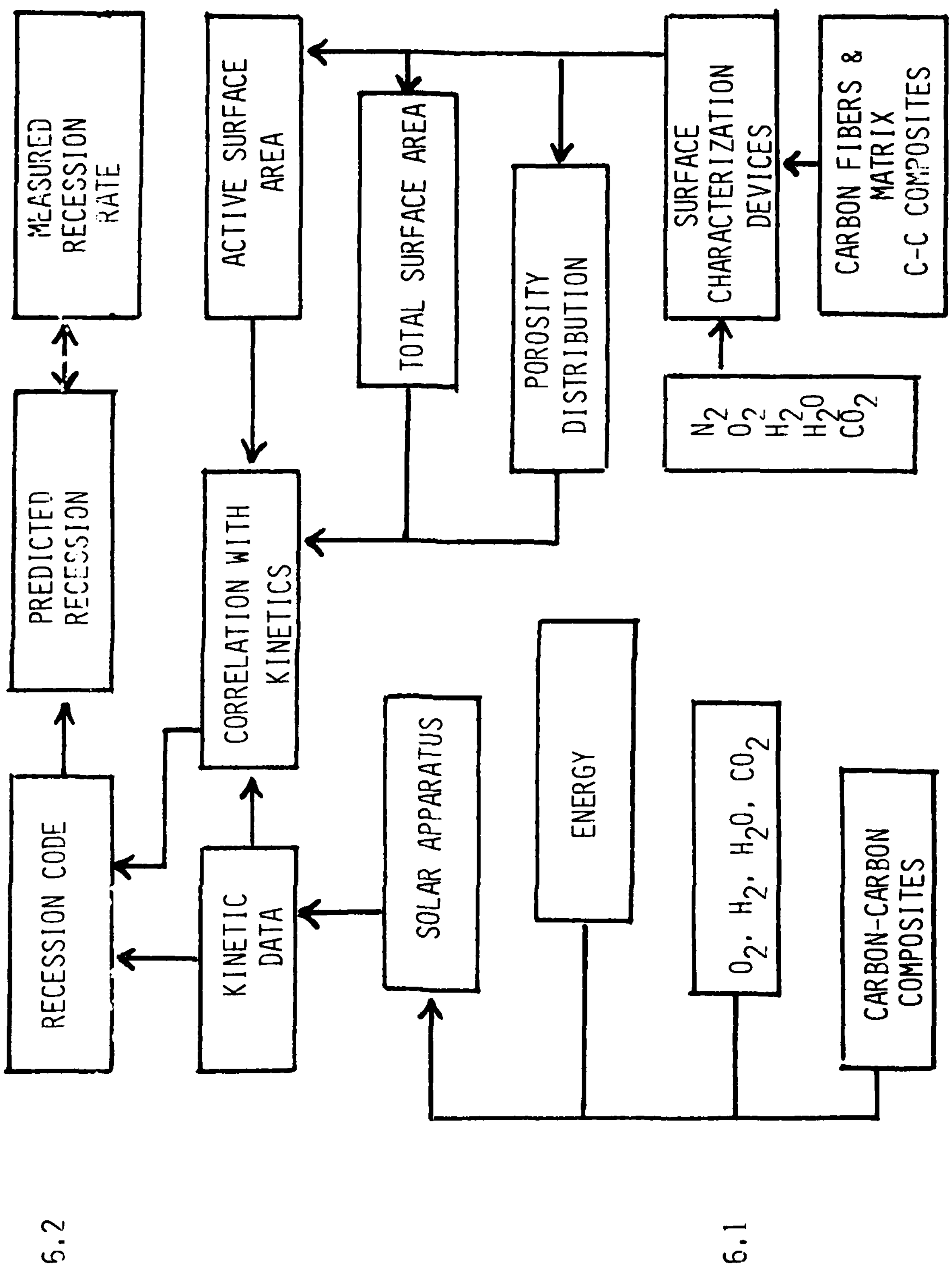

FIGURE 1

ANTICIPATED ACCOMPLISHMENT

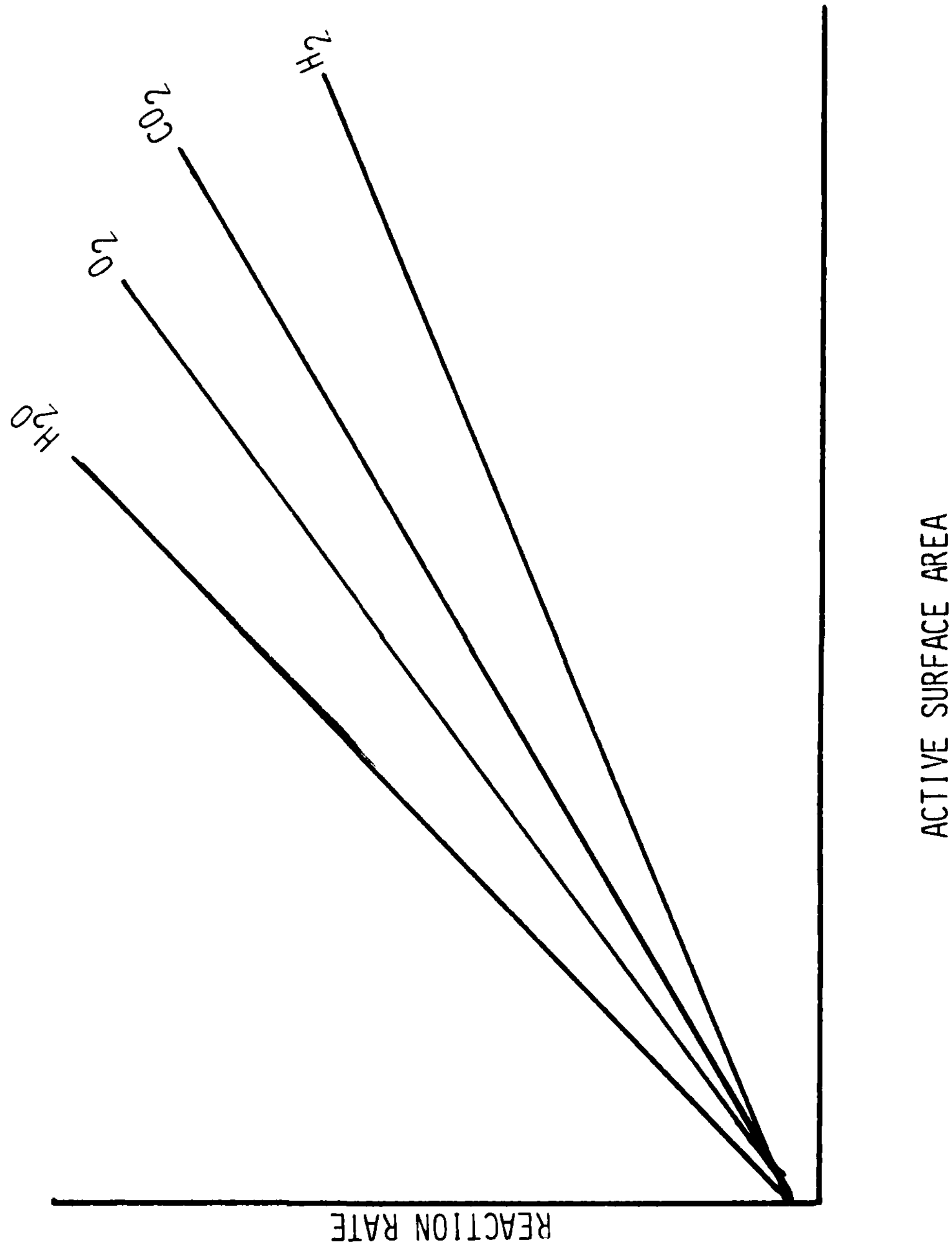

FIGURE 2

METAL COMBUSTION KINETICS

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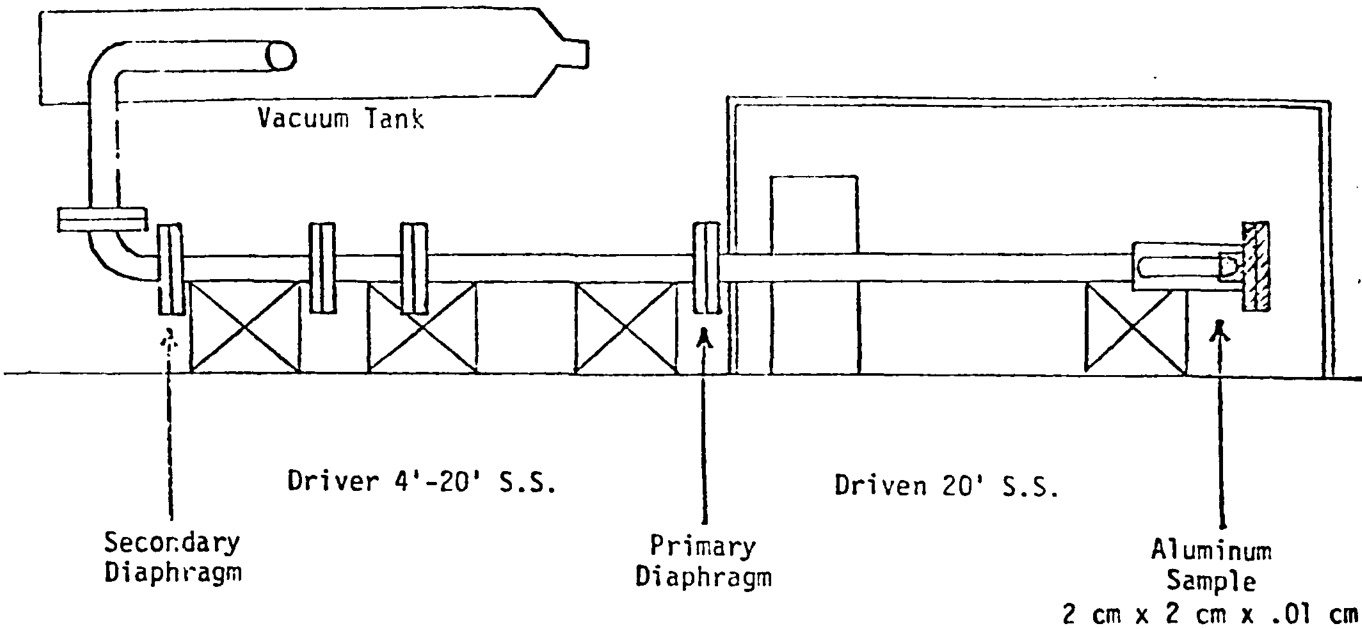
The addition of aluminum to solid propellants for rocket motors can result in significantly improved rocket performance; however, the alumina particulates formed may increase plume visibility, radiative heating of the nozzle and two phase flow losses. While much has been learned about the combustion of aluminum in previous studies, more research needs to be done at elevated temperatures and pressures.

The goal of this project is to obtain data that will help identify the exact reaction mechanism, including intermediate species, and the ignition limits of aluminum at elevated temperatures and pressures. Formidable problems can arise when attempting such measurements in actual rocket motors since the pressures, temperatures and the reaction surface are unsteady and not easy to control. Therefore, it was decided to mount a pure aluminum sample to the end wall of a shock tube and to ignite the sample using a reflected shock wave. The pressures and temperatures that can be achieved (40 atm, 5500^{o}K) are typical of rocket motor conditions and are much higher than those obtained in previous studies using incident shockwaves in conventional shock tubes. Pressures and temperatures can be accurately controlled and measured. The aluminum sample reacts with a test gas in which the proportions of nitrogen, hydrogen, oxygen and chlorine are the same as found in ammonium perchlorate.

During this project the single pulse shock tube shown in Fig. 1 was designed and constructed; proper techniques to carefully ignite the aluminum were determined. The reaction surface was photographed using a high speed movie camera. Recent efforts have resulted in the identification of a number of intermediate species from emission spectra, as seen in Fig. 2. Solid products have been identified using electron diffraction techniques and have been photographed using an electron microscope.

CHEMICAL KINETIC SHOCK TUBE



Aluminum Ignition/Combustion at 40 atm, 5500^o K
Using The University of Michigan Chemical Kinetic Shock Tube

— Test Gas = N_2, H_2, O_2, Cl_2 in ratios corresponding to to ammonium perchlorate

— pressures, temperatures typical of solid rocket motors (much higher than in conventional shock tubes)

— diagnostics: emission spectroscopy
electron diffraction analysis
electron microscope
gas sample analysis

FIGURE 1

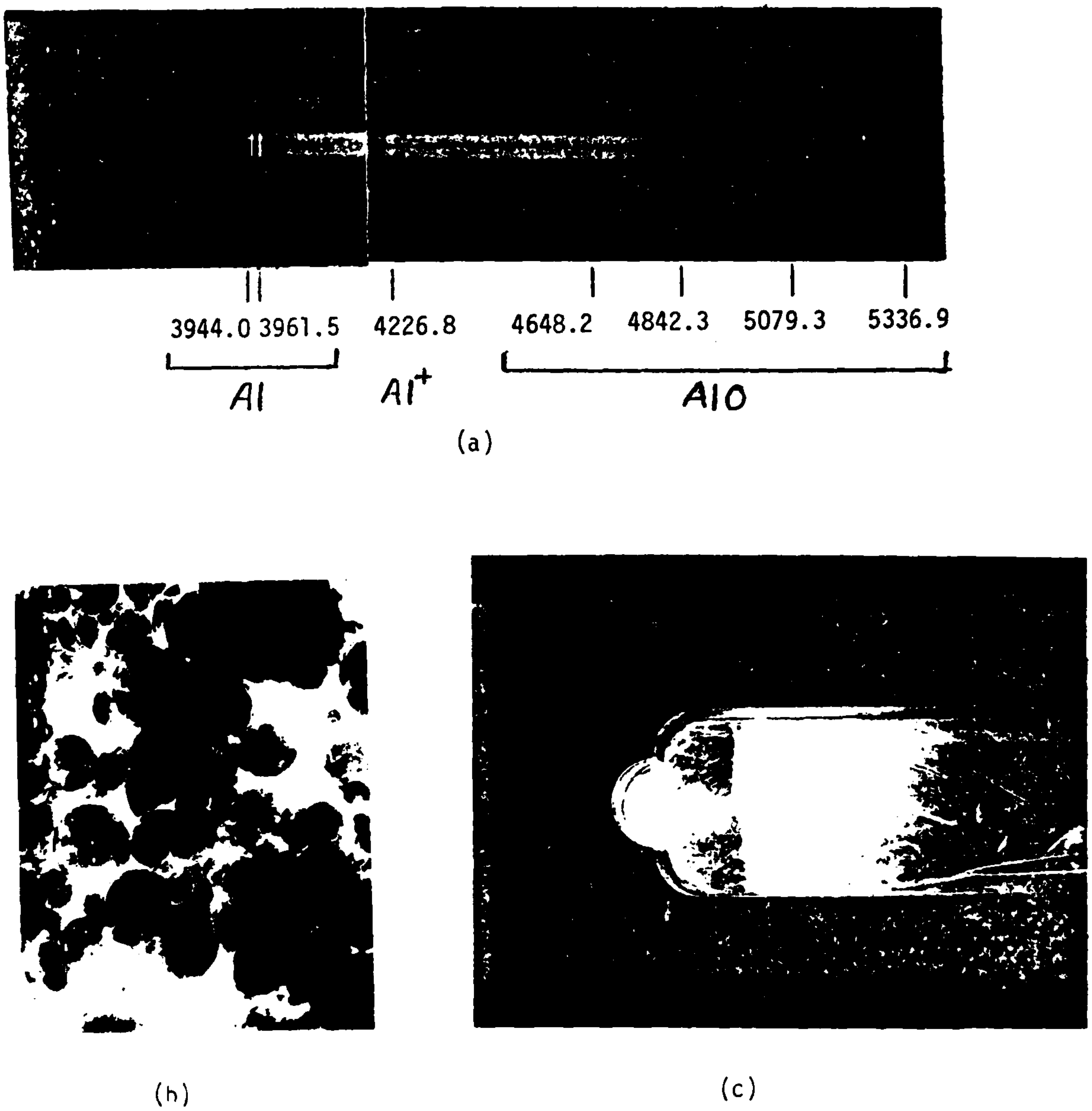


Figure 2. Photographs of:

(a) Typical Emission Spectrum
(b) Micrograph of Products
(c) Ignition Process

THERMOPHYSICAL PROPERTY DETERMINATIONS USING ANSIENT TECHNIQUES

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THERMOPHYSICAL PROPERTIES RESEARCH LABORATORY
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This program involves the use of transient techniques to accomplish two objectves, namely (1) explore thermophysical properties of solid rocket propellants at decomposition temperatures and (2) explore heat transfer in carbon/carbon materials subjected to heat pulses. The overall program is shown schematically in Figure 1.

At temperatures below decomposition, thermal diffusivity measurements are being made using the flash technique. This technique has been modified for making the diffusivity measurements at several temperatures as the sample is heated at a constant rate of about 1°C/sec. The software for controlling the data taking and analysis have been developed, and a temperature controller for heating the sample has been built. However, as the sample approaches decomposition, it is too unstable to use this method for measuring diffusivity. An approach presently being developed consists of using a pulsed flat strip method. This approach could permit heating rates of up to 100,000°/sec, thus allowing for measurements at higher temperatures to be made before decomposition occurs. While these results are not expected to be as accurate as those obtained using the 1°C/sec heating rate, they should still be satisfactory.

For carbon/carbon materials the investigation is being made using the flash diffusivity apparatus with both infrared detectors and thermocouples to examine the heat flow in individual fibers as well as the matrix material. When the rear face temperature rise was measured near a fiber bundle the differences between experimentally observed rise curve and theoretical curve were large (Figure 2). In this case no unique values of diffusivity could be obtained. When the rear face temperature rise was measured at locations which were not near fiber bundles, the response curve nearly approached the theoretical model (Figure 2). In these cases, diffusivity values calculated using longer times (data near the top of the curve) approached a limiting value. It was found that the degree of mismatch between the normalized experimental rise time curve and the theoretical model depends upon three parameters, namely (1) the relative magnitudes of the diffusivity values of the fiber reinforcement and the matrix, (2) the thickness of the sample and (3) the rear face of the sample sensed by the temperature monitor. When the sample is reasonably thick or the ratio of diffusivity values for fiber and matrix appraoch one, then the response curve approximates the theoretical model for a homogeneous material. In this case the diffusivity values calculated at increasing percent rise times asymptotically approach limiting values and these values correspond to the diffusivity values which would be calculated from measured conductivity values.

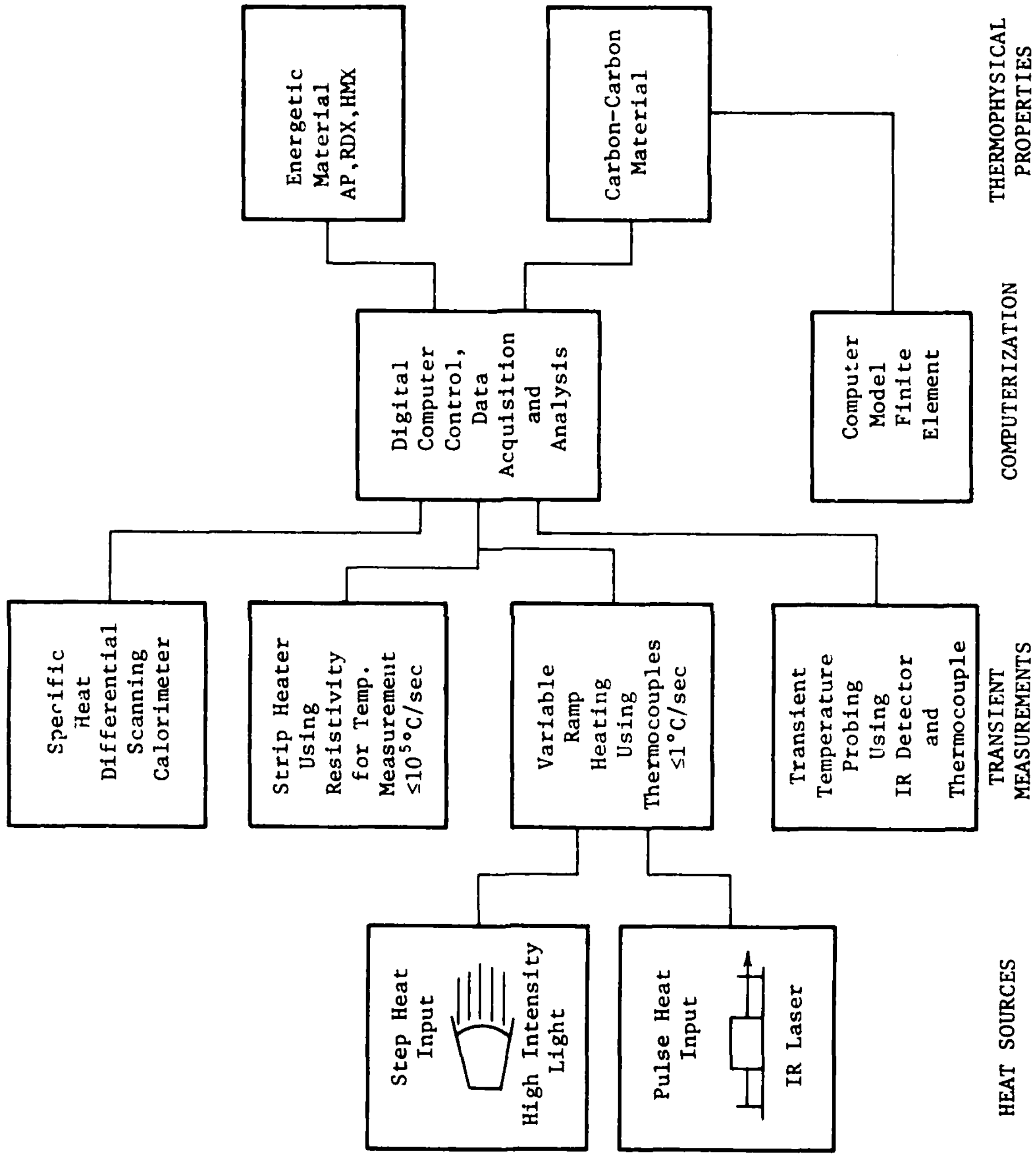

FIGURE 1. THERMOPHYSICAL PROPERTY DETERMINATIONS USING TRANSIENT TECHNIQUES

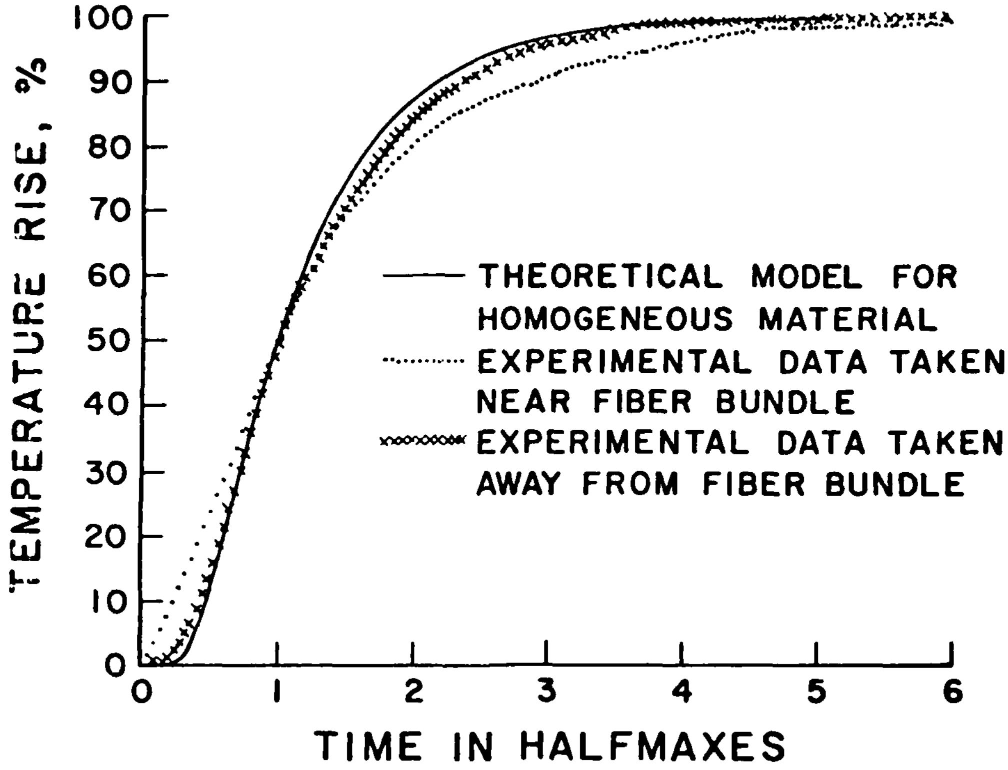

FIGURE 2. NORMALIZED REAR FACE TEMPERATURE RISE CURVES FOR LOCATIONS NEAR AND AWAY FROM FIBER BUNDLES.

HIGH ENERGY PROPELLANT MATERIALS RESEARCH: A TECHNICAL ASSESSMENT

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Menlo Park, CA 94025

Contract: F49620-81-K-0013 Term: 30 June 81 to 29 June 82

Objective: The objectives of the program are to perform a technical assessment of research needs in high energy propellant materials and to identify technological barriers, in terms of propulsion systems requirements, that may require basic research to meet the goals of future solid propellant programs.

Scope: The program includes three tasks: (1) Enumerate current and projected problems in solid propellants that need to be addressed and rank them according to their relevance to Air Force objectives; (2) Assess the applicability of any past and current research to these problems; and (3) Identify potential new research areas that may be beneficial to the development of high energy propellant materials.

Problems associated primarily with three classes of solid propellants are being addressed (See Figure 1): those used for tactical minimum/reduced smoke, orbital insertion and space maneuvering missions. Although not within the scope of this study, materials problems in other propellant applications are being revealed.

Primary sources of data for this study include (1) personal interviews with individuals in the propellant community, (2) accounts of past and current research, and (3) agency program summaries (See Figure 2).

Current Status: The personal interviews are near completion, and the data gathered are being categorized and priorities of identified problems established. Program summaries are being assembled and categorized according to research needs being addressed. The overview presented here highlights our preliminary findings.

Abstract 29
Page 2

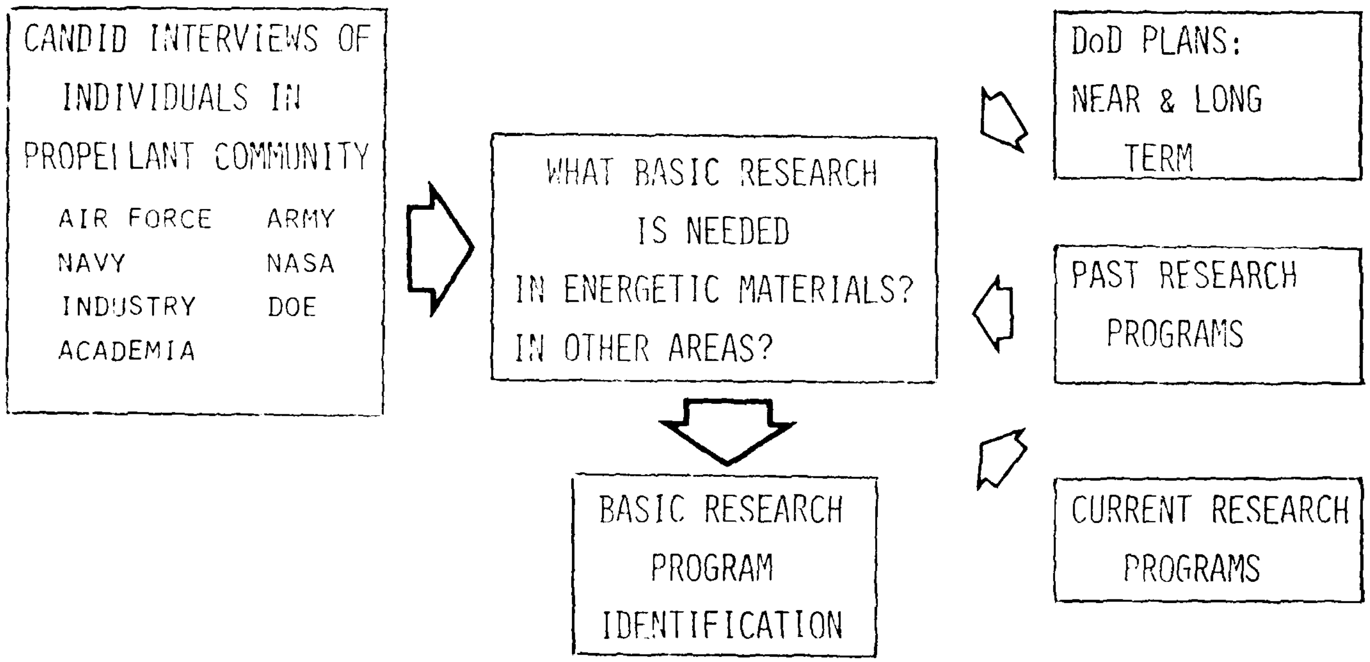
FIGURE 1

BASIC RESEARCH IN ENERGETIC SOLID PROPELLANT MATERIALS:
WHAT IS NEEDED?

MISSILE SYSTEM IN QUESTION	GENERAL PROBLEM AREAS	PROPOSED SOLUTIONS?
• TACTICAL LOW/MIN SMOKE	• PERFORMANCE	• IMPROVED COMMUNICATION
• ORBITAL INSERTION	• HAZARDS	• IMPROVED COORDINATION TO USE RESOURCES BFTTER
• SPACE MANEUVERING	• SIGNATURE	• RESEARCH IN SELECTED KEY PROBLEMS
• OTHER	• ENVIRONMENT	• INCREASE FUNDING
	• AGING	
	• INGREDIENT COST/SUPPLY	

FIGURE 2

PROGRAM INTERACTIONS



NEW SYNTHETIC TECHNIQUES
FOR ADVANCED PROPELLANT INGREDIENTS:
SELECTIVE CHEMICAL TRANSFORMATIONS AND NEW STRUCTURES

Scott A. Shackelford

Air Force Rocket Propulsion Laboratory
Edwards AFB CA 93523

New chemical reaction transformations will be investigated and characterized. Chemical transformations will be considered which lead to energetic target compounds with new or novel chemical structures, or which could lead to improved synthetic routes for known compounds that currently are expensive propellant luxuries. Four tasks will be addressed.

Task 1 involves the use of triflate salts to generate key precursor triflate ester compounds for the subsequent facile introduction of key energetic groups. Silver triflate reacts with some alkyl halides to achieve triflate ester intermediates; however, the scope and limitations of this reaction have not been systematically investigated. Silver triflate reactions with various alkyl bromide structures will be conducted and the reaction scope will be systematically elucidated. In some cases, copper, mercury, and lithium triflates as well as selected alkyl iodides and chlorides will be included.

Task 2 addresses the potential use of both energetic and nonenergetic triflate esters for the direct introduction of energetic moieties into selected organic structures. Past work with triflic anhydride and mixed triflate anhydrides (i.e., trifluoroacetyl triflate) strongly suggests that energetic triflate esters (i.e., 2,fluoro-2,2-dinitroethyl triflate) could introduce energetic groups into selected organic molecules in one step and provide some novel chemical structures. A systematic investigation in various solvents with nonenergetic triflate esters for the introduction of selected anions (i.e., NO_2, F, CNO, N_3) or for reaction with energetic reagents other than alcohols should prove useful.

Task 3 covers the selective fluorination of organic compounds with xenon difluoride. Solid XeF_2 has proved to be a selective, safe, and easily handled fluornation reagent in a few relatively new investigations with alkenes. The scope mechanism, and selectivity of XeF_2 fluorination will be investigated with key multiple bond moieties, whenever appropriate, anionic, aromatic, and saturated aliphatic compounds would be included. Various chemical catalyzed (i.e., Lewis Acids, Lewis Bases, Metal salts) and light initiated (i.e., photochemical, laser) fluorinations will be considered.

Task 4 is concerned with the synthesis and characterization of energetic borazines. Although a few nonenergetic borazine compounds are known, energetic borazines represent a totally new compound class which might find use as propellant oxidizers or burn rate catalysts. Borazine analogs of TATB and TNB plus nonaromatic analogs of compounds like RDX could be interesting ingredients. Polynitoaliphatic or partially fluorinated borazine derivatives will also be considered.

These four tasks address the planning elements required for an effective program: (a) new or novel synthetic transformations, (b) improved synthetic routes, and (c) new target compounds. Other individuals conducting these studies will be Lt Tracy D. Wilson, Ms Lisa J. Emanuel and Lt Steven P. Herrlinger.

APPROACH

SELECTIVE SYNTHETIC TRANSFORMATIONS ⟶ * NOVEL STRUCTURES
* IMPROVED SYNTHETIC ROUTES
* NEW TARGET COMPOUNDS

TASK 1: TRIFLATE SALTS (Selective Intermediate Synthesis)

Alkyl Halide + Triflate Salt ⟶ Key Alkyl Triflate Intermediate® + Metal Salt ↓

Halide = Br, I, Cl   Salts = Ag, Cu, Hg, Li

Task 2: TRIFLATE ESTER INTERMEDIATES (Direct Energetic Structure Synthesis)

Energetic Triflate Ester + Alkyl Compound ⟶ Energetic Alkyl Compound®

Alkyl Triflate Intermediate + Energetic Compound or Selected Anion ⟶ Energetic Alkyl Compound® or Useful Intermediate®

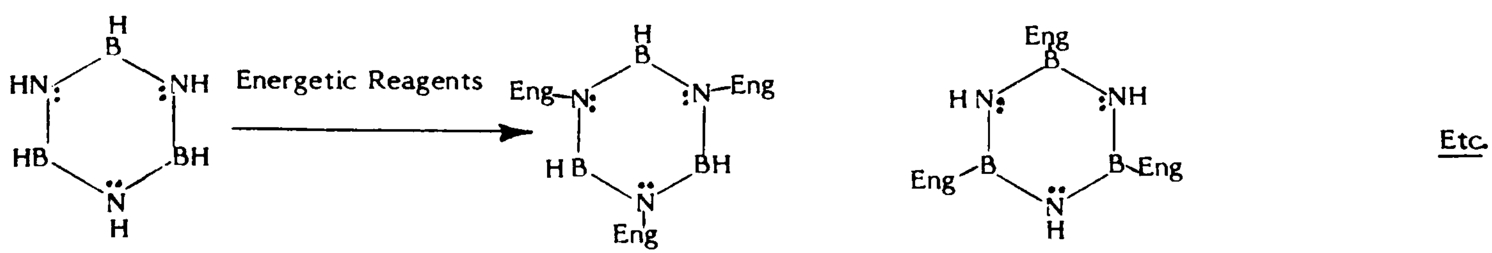
Energetic Triflate Ester Group = Polynitroaliphatic or Nitro Moiety

Task 3: XENON DIFLUORIDE FLUORINATION (Selective Fluoride Synthesis)

Alkyl Compound + XeF_2 ⟶ Specific Alkyl Fluoride or Difluoride

- Chemical Catalysis = Metal Salts/Lewis Acids/Lewis Bases
- Light Initiation = Photochemical Lamp/Laser

Task 4: ENERGETIC BORAZINES (New Compound Class Synthesis)



Eng = Energetic Groups

FIGURE 1

POTENTIAL RESULTS

TASK 1: <u>TRIFLATE SALTS</u> (Improved Selective Synthetic Routes)

- 1° Halides RCH_2X + Ag OTf $\xrightarrow{\Delta}$ RCH_2OTf
- 2° Halides $RCHXCH_3$ + Ag OTf $\xrightarrow{R.T.}$ $RCH(OTf)CH_3$
- $1^{\circ}/2^{\circ}$ Halides $RCHXCH_2X$ + Ag OTf $\xrightarrow{R.T.}$ $RCH(OTf)CH_2X$ (Preferential Displacemen
- Alkenes $>C=C<$ + 2Ag OTf $\xrightarrow{I_2}$ $-C(OTf)-C(OTf)-$ or $>C=C(OTf)-$

TASK 2: TRIFLATE ESTER INTERMEDIATES (Novel Structures/Improved Synthetic Routes)

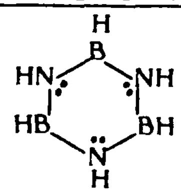
- Ketones or Epoxides + Eng-OTf $\longrightarrow$ R-CH(OEng)-CH(OTf)-R or R-C(OEng)=CH-R
- Alkenes + Eng-OTf $\longrightarrow$ R-CH(Eng)-CH(OTf)-R or R-C(Eng)=CH-R
- Alkyl-Li + Eng-OTf $\longrightarrow$ Selective Energetic Alkyl Compounds
- Alkyl Triflate + HN-$(Eng)_2$ $\longrightarrow$ $RCH_2N(Eng)_2$ (Energetic Compound)

(Eng=Energetic Group) or + X^- $\longrightarrow$ RCH_2X (Useful Intermediate)

TASK 3: <u>XENON DIFLUORIDE FLUORINATION</u> (Novel Fluoride Structure/Improved Synthetic Routes)

- $-C(=O)-$ + XeF_2 $\longrightarrow$ $-CF_2-$ (Geminal Difluorides)
- $RCH=CH_2$ + XeF_2 + EngOH $\longrightarrow$ $RCHF-CH_2OEng$ (Fluorinated Energetic Alkanes)
- Organic Compounds $\xrightarrow{XeF_2}$ $\xrightarrow{\text{Chem. Cat.}}$ Fluoroorganic Ionic Reaction Products; $\xrightarrow{\text{Light}}$ Fluoroorganic Free Radical Reaction Products

TASK 4: <u>ENERGETIC BORAZINES</u> (New Target Compounds)



$(BH-N)_3H$

or

$(BH-N)_3$-NO_2; $-N(FDNE)_2$, -OFDNE, -ODNP, F

$(NH-B)_3$-NO_2; $-N(FDNE)_2$, -OFDNE, -ODNP, F

FDNE = 2-fluoro-2,2-dinitroethyl
ODNP = 2,2-dinitropropoxy

FIGURE 2

MECHANISTIC STUDIES OF NITRAMINE AND ADVANCED PROPELLANT INGREDIENT INITIAL THERMOCHEMICAL DECOMPOSITION
2303 MI SN

Berge B. Goshgarian

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This research program is directed toward the understanding and elucidation of thermochemical initiating, rate-determining, and propagating reaction steps of propellant ingredients and the systematic correlation of the data to ingredient molecular structure. Results will assist in improving propellant combustion tailoring, mechanical and physical properties, and propellant performance predictions. Mechanistic elucidation/molecular structure correlation will also guide in the synthesis of advanced propellant ingredients possessing desirable properties. The initial and rate-determining thermochemical reaction steps, mechanisms, and kinetics of propellant ingredients and mixtures will be elucidated using a variety of analytical techniques and isotopically labeled compounds. Data will be acquired under a variety of thermal conditions including heating rates up to 20,000 degrees centigrade per second and pressures from zero to 130 atmospheres. The Arrhenius parmeters and initial and final thermochemical decomposition products of glycidyl azide polymers (GAP) and gumstocks were obtained during this reporting period. The initial decomposition step is the rupture of the RCH_2N-N_2 bond to form nitrogen by first order kinetics. The rate equation for this process, based on the evolution rate of nitrogen from thermally decomposing GAP is $k = 2 \times 10^{14} e^{-38,000/RT} (sec^{-1})$ (509-525K). Some ammonia and hydrazoic acid are also formed during initial decomposition. Secondary processes include rupture of carbon-carbon, carbon-hydrogen, and carbon-oxygen bonds in the polymer backbone. An average rate equation for these processes, based on the evolution rate of carbon-containing products from thermally decomposing GAP is $k = 10^{21} e^{-58,000/RT} (sec^{-1})$(509-525K). The secondary decomposition processes produce ethylene, methane, ethane, hydrogen, propene nitrile, acrylaldehyde, 2-imino ethanal, and carbon monoxide as major products. A rate equation based on the change in rate of condensed phase heat release, which includes all processes occurring in the condensed phase during GAP thermochemical decomposition is $k = 7 \times 10^{15} e^{-42,400/RT} (sec^{-1})$ (520-540K). Glycidyl azide polymer gumstocks produced nearly identical thermochemical decompositions products as the polymers. Their average rate equation, based on the change in rate of condensed phase heat release is $k = 2 \times 10^{13} e^{-36,400/RT} (sec^{-1})$ (520-540K).

Le Ann Lindsay and Gayle Angelo were assigned to this program during the GAP studies. Capt Scott Shackelford and Lt Mike Collidge are presently assigned for the remainder of the program.

ISSUES	APPROACH	RESULTS
MECHANISM Identify initial/rate-determining thermochemical decomposition reaction steps and mechanisms of propellant ingredients.	*Identify primary and secondary products from controlled thermochemical decomposition. *Isotopically label ingredients to determine reaction mechanisms. *Deuterium isotope labeling to identify reaction rate-controlling bond rupture.	*Improved techniques for predicting, controlling and improving propellant performance. *Combustion tailoring. *Longer-term storage life. *Improved propellant mechanical properties. *Better ingredient synthesis.
KINETICS Acquire thermochemical kinetic parameters of propellant ingredients.	*Determine reaction rates, activation energies, pre-exponential factors under variety of temperature, pressure, and thermal rate conditions. * Measure change in reaction rate by deuterium isotope effect (to identify rate determining step). *Determine temperatures where free radicals form. *Identify catalysts/additives that will modify thermochemical properties. *Develop high pressure-high heating rate analytical technique for acquisition of kinetic parameters.	

FIGURE 1

GLYCIDYL AZIDE POLYMER & GUMSTOCK
THERMOCHEMICAL DECOMPOSITION PROPERTIES

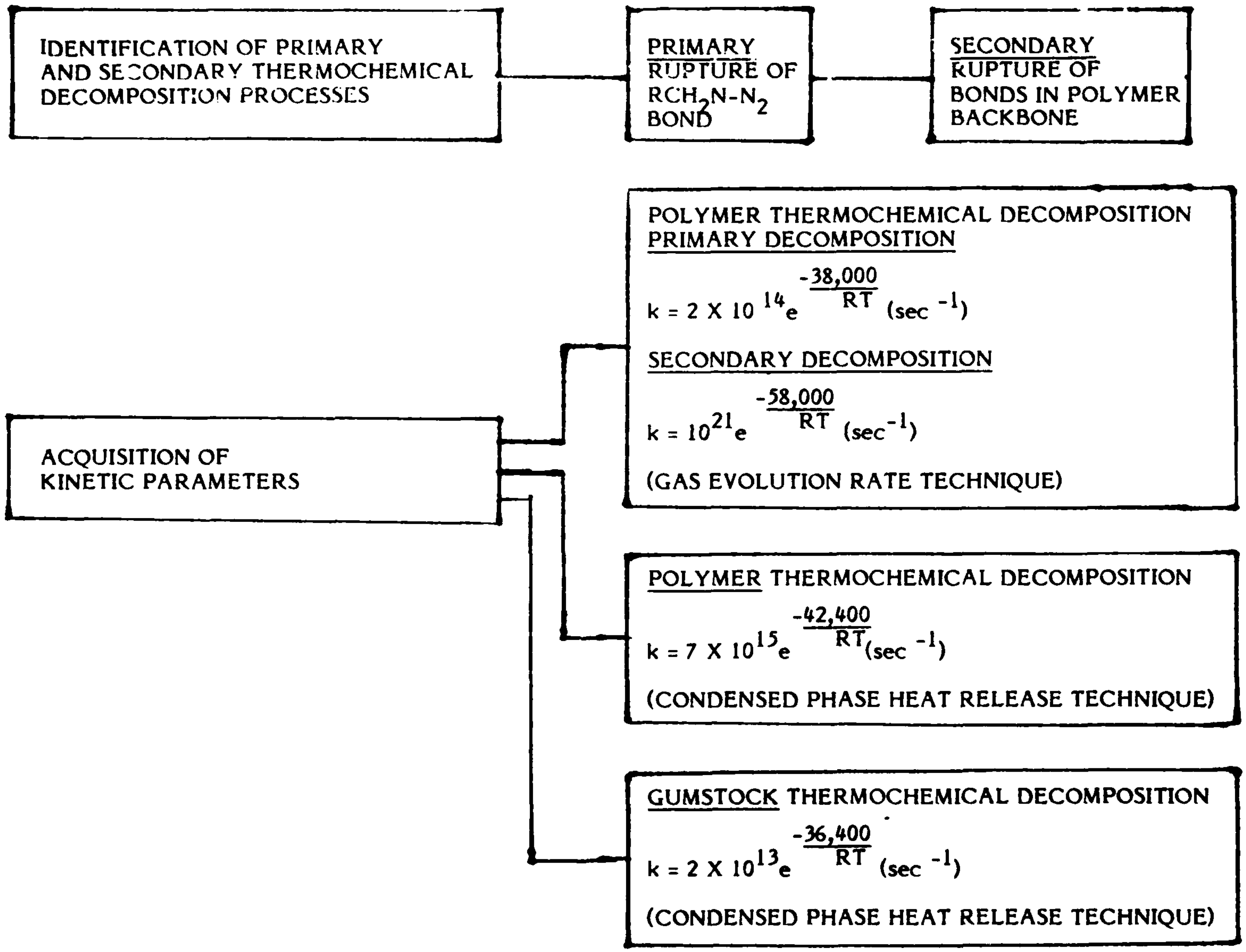

FIGURE 2

I. Synt'..sis of Hydroxy-Terminated Dinitropropyl Acrylate Polymers

II. Improved Characterization of Hydroxy-Terminated Prepolymers

F 04611-79-C-0009/P00006

C. Sue Kim

California State University, Sacramento
Sacramento, California

I. Dinitropropyl Acrylate (DNPA) polymer with hydroxyl functionality of 2.8 was synthesized. The polymer is such that both ends of the chains are terminated by primary alcohols as much as possible and a secondary alcohol is incorporated along the chain. These DNPA polymers have potential as co-prepolymers or crosslinkers to be used along with polyethylene glycols or polycaprolactones. It is hoped that these combinations give improved compatibility with the nitro or nitrato-plasticizers without sacrifice of the mechanical properties.

II. Characterization methods of propellant prepolymers involving determinations of hydroxy-equivalent weight, molecular weight, and functionality are being examined. In this connection, a new technique for equivalent weight determination was developed based on the strong absorption band of the tetrahydrofuran-associated hydroxyl groups in the 3450 cm^{-1} infrared region. This method was evaluated in terms of various factors which may influence the quantitative aspects of this technique. The detailed study is being published in the February issue of Analytical Chemistry.

FIGURE I: APPROACH

I. Synthesis of Hydroxy-Terminated DNPA Polymers

(A) Free-Radical, Solution Polymerization - Study Kinetics and Mechanism

(B) Optimization of Polymerization Conditions To Improve Functionality

II. Improved Characterization of Hydroxy-Terminated Prepolymers

(A) Equivalent Weight Determination (EW)

(1) NMR Method - evaluate

(2) IR Method - develop and evaluate

(3) Chemical Methods - evaluate

(B) Molecular Weight Determination (MW)

(1) Vapor Phase Osmometry - evaluate

(2) GPC-Viscosity Combination Method - develop and evaluate

(C) Functionality Determination (f)

(1) f = MW/EW - evaluate

(2) "Cure" Method Based on $\sum_{n=1}^{n} \frac{(f_i-2)e_i}{f_i} = 0$ - evaluate

FIGURE II: ACCOMPLISHMENT

I. Hydroxy-terminated DNPA polymers, f = 2.8 or higher, were synthesized.

Potential Applications: Copolymer and Crosslinker in the Energetic Binder Systems.

II. Characterization Methods

(A) Equivalent Weight Determinations

(1) IR method was developed

(2) Advantages and limitations of three methods, IR, NMR and chemical, were analyzed.

(B) Molecular Weight Determinations

(1) GPC-Viscosity combination method is being developed.

(2) Vapor phase osmometry was evaluated.

(C) Functionality Determinations

(1) Two methods, f = M.W./E.W. and "cure" method, are being evaluated.

Structure-Property Relationships in Polyether Elastomers

Stan Morse

University of Dayton Research Institute
Research Performed at the Air Force Rocket Propulsion Laboratory

This research is a continuation of work started last year which involves the study of chemical changes made in a polyether prepolymer (low molecular weight, liquid polymer) and the effect of these changes on the physical-mechanical properties of elastomers made from these prepolymers. The fundamental questions deal with the change in the mechanical properties of a rubber (elongation, tensil strength, etc.) with the addition of internal crosslinks to a polymer network which is primarily an end-linked network.

The approach of this work has been the study of the polymerization of epoxides to obtain liquid polyethers that will cure into a rubber. Previously we reported on the study of acid catalyzed polymerization of epichlorohydrin and the copolymerization of epichlorohydrin and a diepoxide. From these liquids, elastomers have been made by a diisocyanate end-linking reaction. The physical-mechanical properties of these rubbers have been measured. The addition of diepoxides to epoxide polymerizations is not new. Resins and elastomers have been modified by this method but there is little in the literature about this modification to prepolymers for end-linking reactions.

From the prepolymers gumstocks were formed by diisocyanate cure. In all cases the modulus and tensil strength was higher for the elastomer that contained the modified prepolymer than for the elastomer made from the unmodified prepolymer. The elongation for those elastomers was lower as would be expected for increased crosslinking in the network. A spectrum of mechanical properties can be obtained from these polymers when the crosslinking of the diepoxide is varied.

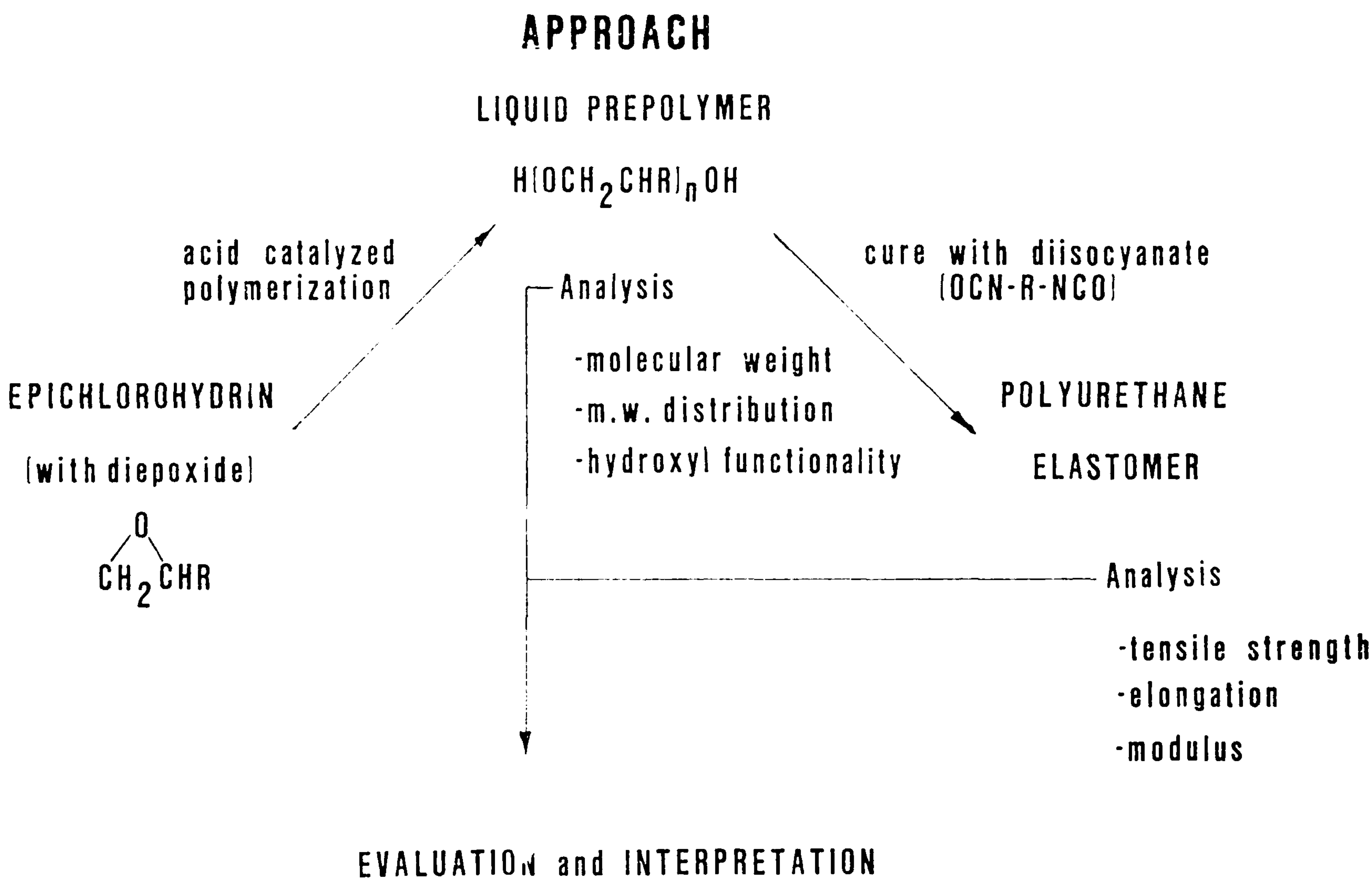
APPROACH
LIQUID PREPOLYMER
H(OCH2CHR)nOH
acid catalyzed polymerization
EPICHLOROHYDRIN
(with diepoxide)
O
CH2CHR
Analysis
-molecular weight
-m.w. distribution
-hydroxyl functionality
cure with diisocyanate (OCN-R-NCO)
POLYURETHANE
ELASTOMER
Analysis
-tensile strength
-elongation
-modulus
EVALUATION and INTERPRETATION

FIGURE 1

ACCOMPLISHMENTS

- Increased understanding of structure-property relationships

- Method for varying mechanical properties

- Method for varying elastomer formation characteristics

KINETICS AND THERMODYNAMICS OF THE $\beta\rightarrow\delta$ HMX TRANSFORMATION: AN APPROACH TO ALTERING THE NATURE OF HMX

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Newark, Delaware 19711

The purpose of this research is to determine and measure the thermodynamic and kinetic events that take place on a molecular level in the condensed phase of nitramines. This information is needed to characterize the chemical and mechanical properties of monopropellants in which phase changes and dynamic processes are important. A recently embarked upon program which has developed from these molecular dynamics studies involves the modification of HMX decomposition and burn rate by dopants tailored specifically for the HMX crystal lattice.

The thermodynamics of the $\beta\rightarrow\delta$-HMX phase transition has been solved by using laser Raman spectroscopy and high pressure technology developed in our laboratory. The kinetics element is being solved by using Fourier transform (FT), nuclear quadrupole resonance (NQR) and infrared (IR) techniques. The combustion modifications research has begun by employing single crystal X-ray diffraction to determine the size, shape, and electronic characteristics of voids that can be formed in an HMX crystal lattice. Once these voids are parameterized, it should be possible to design metal-containing catalysts possessing structures that can be incorporated in the HMX crystal lattice.

During 1981 the thermodynamics of the $\beta\rightarrow\delta$-HMX phase transition was determined at pressures up to 10^5 psi and temperatures up to 250°C for 3 μm and 175 μm HMX. The $\beta\rightarrow\delta$ phase transition is regular and normal below 30000 psi in 3 μm HMX, but experiences an abrupt slope break above 30000 psi. 175 μm HMX has the same appearance except that the break occurs at lower P and T. The slope breaks result from the onset of decomposition in HMX. The decomposition products are retained to a much greater degree in 175 μm HMX than in 3 μm HMX. Hence 3 μm HMX gives a truer phase diagram below 30000 psi. However 3 μm HMX experiences extensive degradation above 240°C, and 30000 psi. This decomposition produces a severe disruption and expansion of the crystal lattice which allows the $\beta\rightarrow\delta$ transition to occur very easily. ΔH calculated for 3 μm HMX above 245°C is about equal to the activation energy for the decomposition of HMX (250 KJ/mole).

The rate of the $\beta\rightarrow\delta$-HMX transition is being determined by FT-IR and FT-NQR spectroscopy. Preliminary results reveal that the rate of the $\beta\rightarrow\delta$ phase transition is orders of magnitude faster than the burn rate of HMX propellants. Consequently, our thermodynamics and kinetics research both indicate that δ-HMX is the polymorph present in the combustion of HMX.

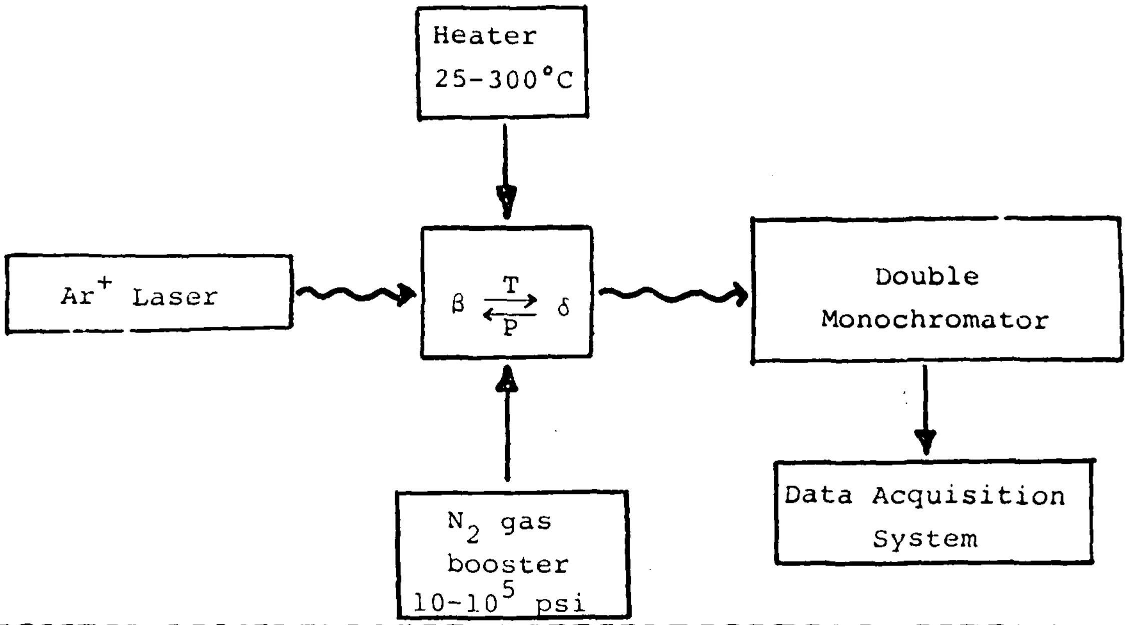
The location of the voids in the HMX crystal lattice and the electrostatically sensitive sites on the HMX molecule involves the use of single crystal X-ray diffraction. The structures of stoichiometric solvates of HMX are being examined now. Knowledge of the interaction sites will allow design of complexes containing metal catalysts which can be incorporated in the HMX lattice.

TECHNICAL APPROACHES

UNIVERSITY OF DELAWARE P. I.: THOMAS B. BRILL

MOLECULAR DYNAMICS IN SOLID NITRAMINES

- PHASE DIAGRAM STUDIES (RAMAN SPECTROSCOPY)



- KINETICS OF PHASE CHANGES (^{14}N NUCLEAR SPECTROSCOPY)

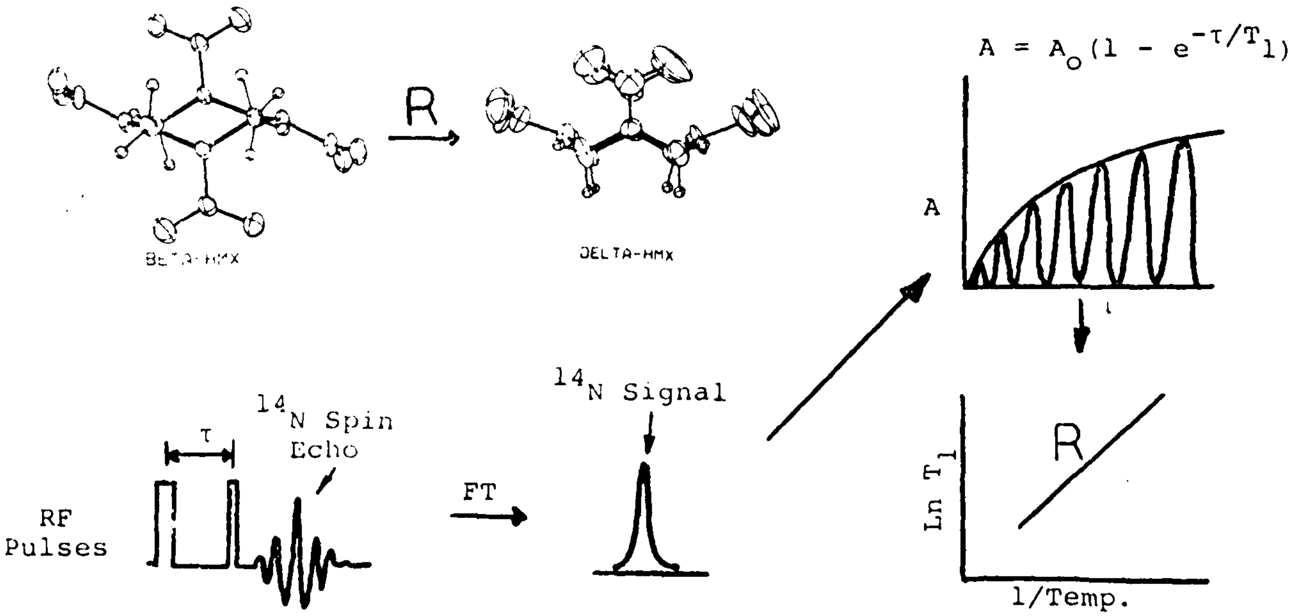


FIGURE I

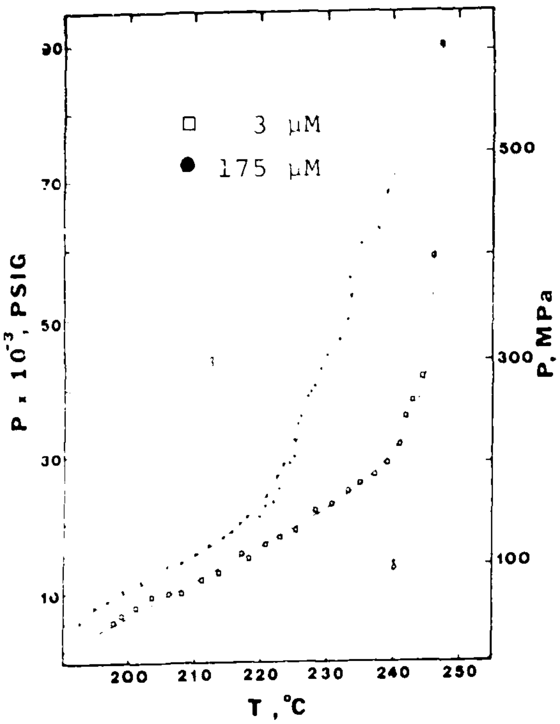
Abstract 34

Page 2

TECHNICAL ACCOMPLISHMENTS (1981)

UNIVERSITY OF DELAWARE

P.I.: THOMAS B. BRILL



THE β→δ HMX SOLID PHASE DIAGRAM

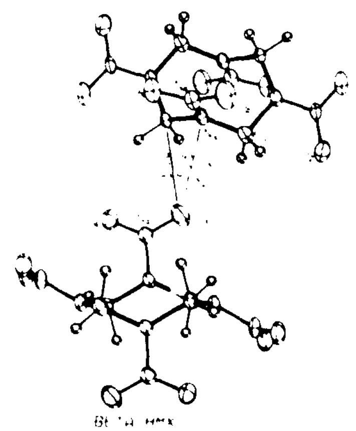
- δ-HMX is the stable polymorph above 248°C regardless of the pressure.
- Enthalpy and Entropy values have been established up to 690 MPa (100,000 psi).
- 3 μM HMX does not retain decomposition products to the extent that larger particle sizes do. Therefore, 3 μM HMX should be used for decomposition studies if mechanistic detail is sought.

KINETICS AND HMX MODIFICATIONS

Fourier transform-IR methods show the rate of the β→δ-HMX transformation is orders of magnitude faster than propellant combustion rates. δ-HMX is therefore the polymorph that initiates decomposition.

The most important intermolecular cohesive force in pure HMX is the O···CNC interaction.

- Motion about this interaction dominates the molecular dynamics of HMX.
- In order to modify HMX by doping the lattice, an interaction of this type must be mimicked.



Primary intermolecular interaction in β-HMX. The O_3 atom of the axial NO_2 groups engages in an electrostatic attraction with C_1 and C_2 and a repulsive interaction with N_3 of a neighboring molecule. (Distances are shown in Å.)

FIGURE 2

Abstract 34
Page 3

AD-A116 080 1982 AFOSR/AFRPL ROCKET PROPULSION RESEARCH MEETING HELD AT LANCASTER CAL..(U) AIR FORCE OFFICE OF SCIENTIFIC RESEARCH BOLLING AFB DC L H CAVENY ET AL. 2/2

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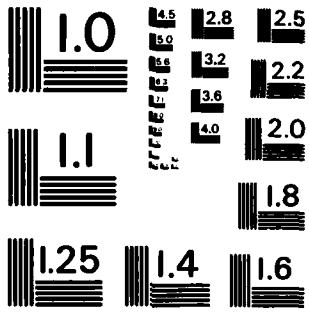
1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
5.6
6.3

HMX COMBUSTION MODIFICATIONS

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Rockwell International
Canoga Park, CA 91304

The rapidly accelerating usage of HMX/RDX for minimum smoke solid propellants has been hampered by a lack of ballistic tailoring flexability which limits the motor design engineers.

The current research effort has several facets which are aimed at correcting the burning rate problem. First, the incorporation of azido moieties has been investigated via: 1) co-precipitation; 2) direct addition as a co-oxidizer; and 3) attempts at the synthesis of cyclic analogs in which the methylazido group ($-CH_2N_3$) replaces the nitro ($-NO_2$) group on the ring nitrogen. Accelerated rates were obtained via methods 1 & 2 in which a linear diazidonitramine (DATH) was employed. However, the rates were the same for both methods.

Attempts at the synthesis of the 6 and 8-membered cyclic nitramines with azido substitution have not been successful. The 7-membered cyclic compound containing one C-C bond has been successful, but partial substitution of this compound did not increase the burning rate.

A variety of compounds which can generate NH_3 and eventually the amidogen radical ($-NH_2$) has been investigated and the burning rate has been accelerated by 250% in a baseline binder based upon R-18/TMETN.

Studies of the role of gas phase kinetics in HMX combustion indicate that gas phase interactions strongly influence, if not dictate the behavior of HMX combustion. To investigate the role of gas phase interactions in HMX combustion, quantitative analyses of gas phase product distributions from HMX and isotopically labeled HMX (ring N^{15}) with and without additives has been investigated. A pyrolysis unit interfaced to a gas chromatograph and mass spectrometer was used in this study. Samples were pyrolyzed within a quartz capillary under 2 atmospheres helium at the maximum heating rate available (~850°C per second).

The products of HMX (ring N^{15}) decomposition just above the melt region (~300°C) are 51 mole percent N_2O, $26N_2$, 18NO, and $2NH_3$ based on total HMX nitrogen. Products based on total HMX carbon are 28 mole percent CH_2O, $19CO_2$, 13CO, and $5CH_4$. In addition, 19 mole percent H_2O (based on total HMX oxygen) was recovered. Mass spectrometer tracer studies show N_2O and N_2 result from primary pyrolysis processes involving C-N bond cleavage without $N-NO_2$ cleavage. NO formation results predominantly from $-NO_2$ nitrogen. HCN formation does not occur in this low temperature region suggesting a rate controlling process.

In the high temperature region (~800°C) NO becomes the major product in HMX (ring N^{15}) decomposition resulting in 42 mole percent NO, $21N_2$, $18N_2O$, and 17 HCN. Products based on total HMX carbon are 35 mole percent HCN, 32CO, $19CO_2$, and less than $5CH_4$. In addition 21 mole percent H_2O (based on total HMX oxygen) was recovered. Tracer studies in the high temperature region show that $N-NO_2$ bond cleavage becomes faster than C-N bond cleavage and that increased NO and decreased N_2O yield is not a result of N_2O gas phase decomposition as might be expected. In addition, it was shown that HCN formation results predominantly from ring nitrogen in HMX.

Gas phase reduction of HMX NO by NH_2 intermediates (from energetic additives) appears to play a key role in modifying HMX combustion. Tracer studies with mixtures of HMX (ring N^{15}) and bistriaminoguanidinium azobitetrazole (TAGZT) have been shown to modify HMX combustion by reduction of HMX NO to N_2 and H_2O by TAGZT NH_3.

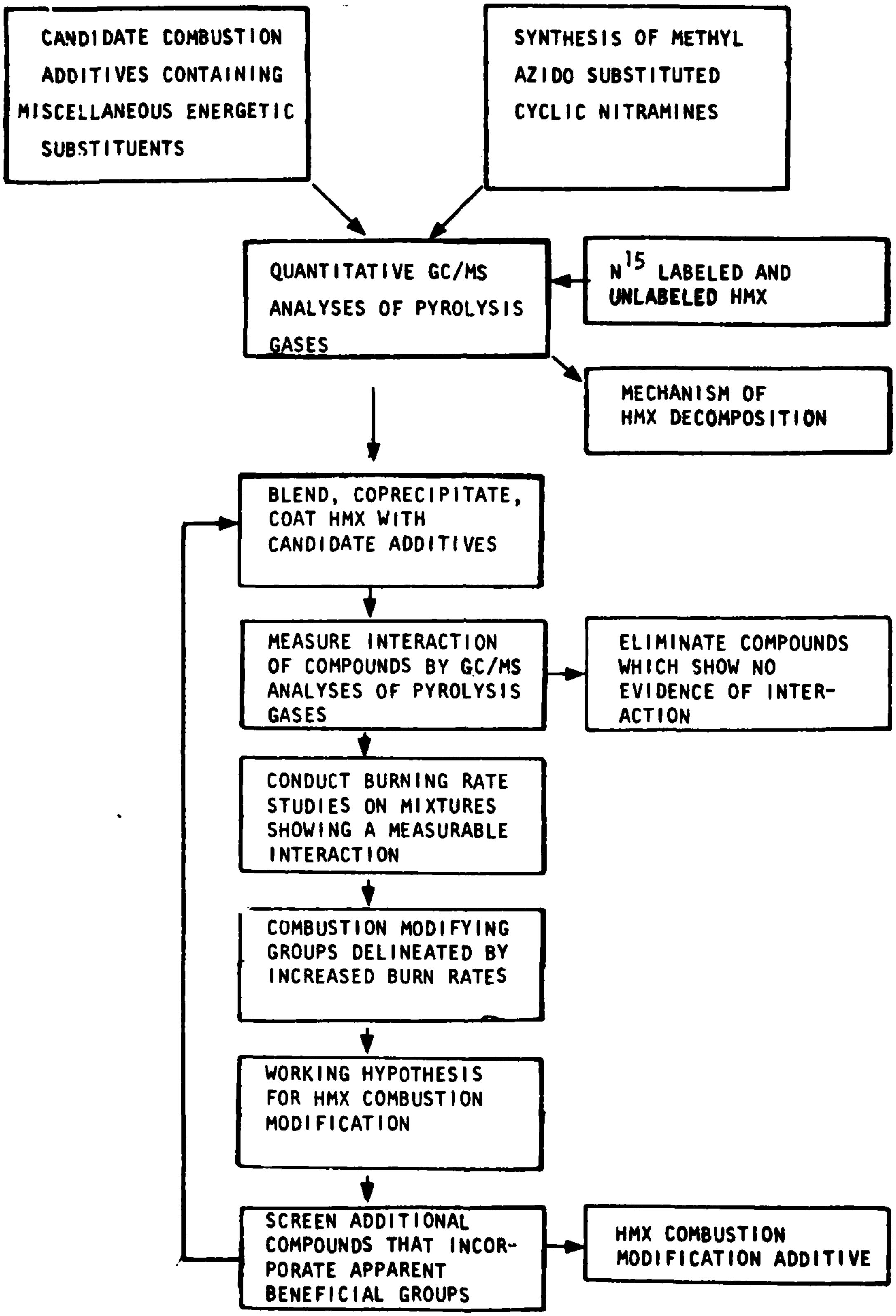
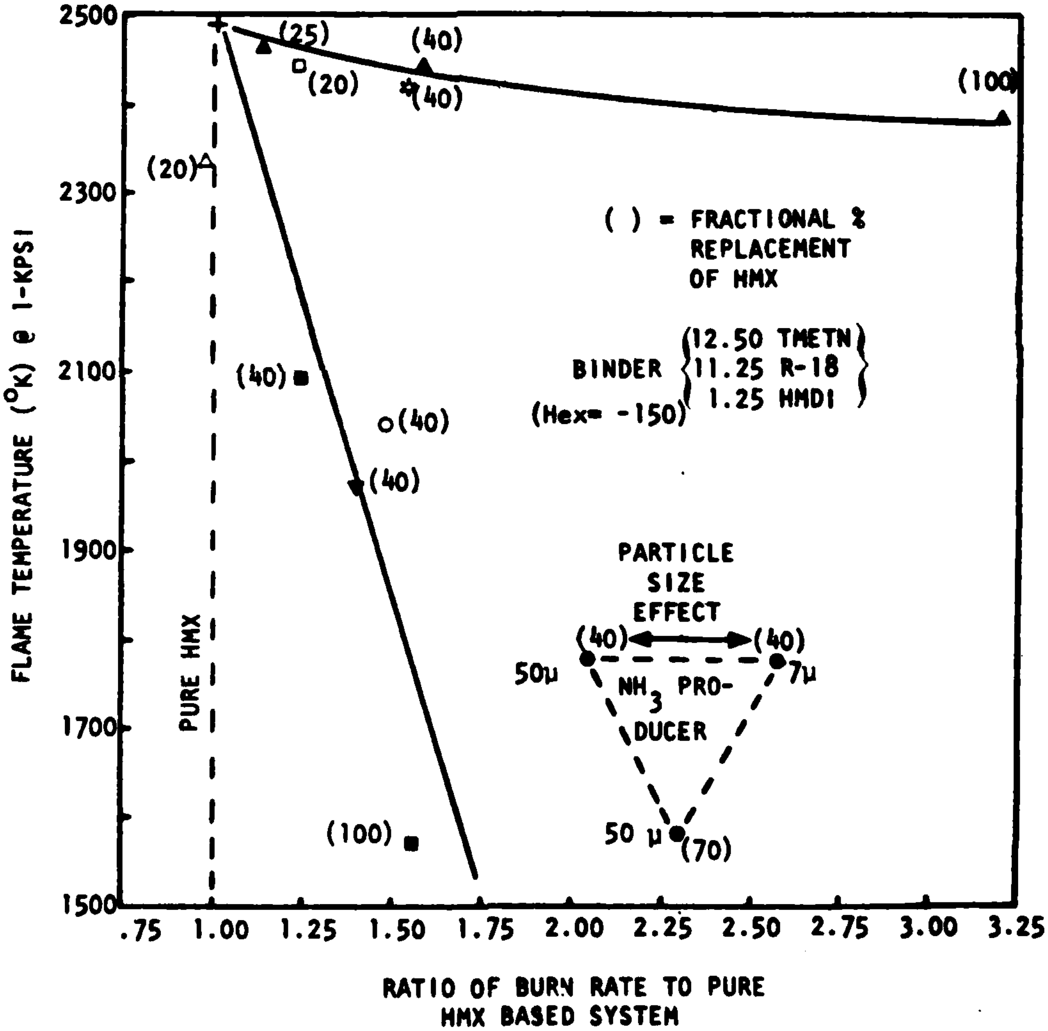


Figure 1. Scientific Approach for HMX Combustion Modification

BURN RATE EFFECTS
75% HMX (1:1-GLASS A/E)

ADDITIVES:

- ● DI-TAG SALT OF BISAZOTETRAZOLE (TAGZT)
- ▲ 1,7-DIAZIDO-2,4,6-TRINITRAZAHEPTANE (DATH)
- ■ TAG-NITRATE (TAGN)
- □ AZOBISNITROFORMAMIDINE (ABNF)
- △ 3-AZIDOMETHYL-1,5-DINITRO-1,3,5-TRIAZACYCLOHEPTANE (AMDTH)
- ✲ HYDRAZINE NITRATE (HN)
- ○ AMMONIUM SALT OF NITRAMINOTETRAZOLE (ANAT)
- ▼ TAG-SALT OF NITRAMINOTETRAZOLE (TAGNAT)



THE VAPOR PRESSURE OF SALT-HCL-WATER SOLUTIONS BELOW OC

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UNIVERSITY OF NEVADA
MACKAY SCHOOL OF MINES

The equilibrium vapor pressures of hydrochloric acid solutions are fundamental to the development of secondary smoke droplets in the plumes of ammonium perchlorate composite solid rockets. Inorganic salts introduced into the propellant formulation as processing aids, burn rate modifiers or contaminants nucleate the condensation of the droplets, dissolve in the acid significantly modifying its equilibrium vapor pressure and composition, and hence modify the character of the smoke.

No vapor pressure data existed for either pure or salted hydrochloric acid solutions below OC before the present work. Extrapolations of data from temperatures above OC were unsatisfactory. Measurements for pure hydrochloric acid solutions have previously been completed. Sodium and calcium chlorides were selected for continued study since they are the major salts present in the rocket plume which impact on the vapor pressure of the hydrochloric acid and the formation of smoke droplets.

As illustrated in Figure 1, the total vapor pressures are measured by means of capacitance gauges for selected solutions in a 2-liter pyrex flask immersed in a methylene chloride bath cooled by a mechanical refrigeration system. Removal of air from the system is accomplished by a mechanical vacuum pump in series with a liquid nitrogen trap. Vapor compositions are determined using a quadrapole mass filter spectrometer (VGA). The salt is separated from an acid solution sample and dissolved in water. Both the pure acid and the salt solutions are then analyzed by means of an electroconductometric bridge.

Figure 2 highlights the progress made during this period. Measurements were completed for the remaining range of acid compositions saturated with sodium chloride for the temperature range of 0 to -40C. Confirmatory tests were conducted for several solutions, as indicated from an evaluation of the data. Studies continue of intermediate concentrations of dissolved sodium chloride. Evidence has been obtained of formation of a sodium chloride hydrate in equilibrium with the saturated acid solutions. This hydrate will cause increased vapor condensation and secondary smoke. The gas analyzer sensitivity factor previously determined from thermodynamic considerations has been confirmed experimentally.

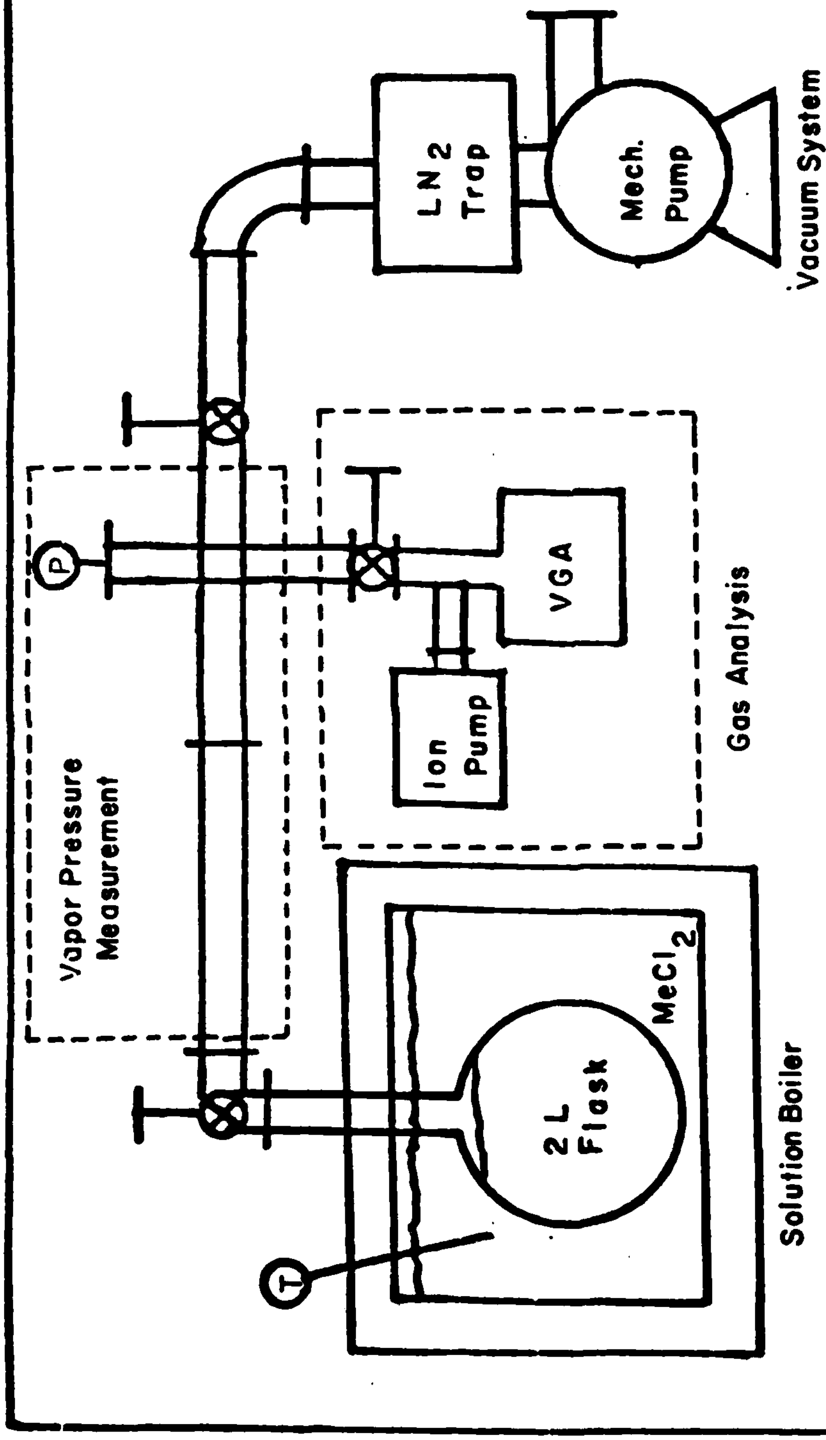

FIGURE 1
Schematic of Experimental Apparatus

- VAPOR PRESSURE MEASUREMENTS COMPLETED FOR HYDROCHLORIC ACID SATURATED WITH SODIUM CHLORIDE FOR:

  7.1 - 34.0 WT PCT ACID
  BETWEEN 0 AND -40C.
  VAPOR PRESSURE HCl HIGHER AND VAPOR PRESSURE H_2O LOWER THAN PURE ACID. ACCENTUATED BY FORMATION OF SODIUM CHLORIDE HYDRATE.

- SALT SOLUBILITIES AND WATER VAPOR PRESSURES LOWER THAN EXTRAPOLATED VALUES USED IN SMOKE MODELS.

- INTERMEDIATE CONCENTRATIONS OF SODIUM CHLORIDE IN ACID SOLUTIONS BEING COMPLETED.

FIGURE 2

FLOW OF GAS-PARTICLE MIXTURES

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Abstract

There are many practical examples of engineering systems in which small, solid particles are mixed with a gas and the mixture flows through the system. The visible trailing plume from a rocket engine is formed in part by burning of small particles flowing from the rocket engine when they mix with the air in the atmosphere. These particles can also collect on the outer surfaces of spacecraft windows and reduce transmission and reception of light used for navigation and scientific data collection. Mixtures of small particles and gases also occur in pulverized coal combustion and gasification, aircraft engines, diesel engines, and woodburning fireplaces and stoves.

Understanding of these flows with gases and particles is necessary to design the systems and predict their performance. For example, how fast the particle burns depends on how far into the surrounding air it moves and how much air it is exposed to. Unfortunately, these flow systems are very complex and poorly characterized even though they occur so frequently. This report summarizes studies being conducted to characterize the flow of a gas particle mixture in a round jet including the characterization of particle interactions with pressure waves formed in the jet in high speed compressible flow. Recently developed systems using light to make the measurements have shown great promise in making these measurements. Recent results of the studies have included measurment of particle location and concentration, velocity, size distribution and shock wave structure for comparison to computation results. The flows of primary interest are nozzle and jet flow with micron-sized particles. Specific measurements in the study are outlined below.

Axial and radial velocity distribution of particles in the round jets and before and after shock waves in the flow are being measured by a laser anemometer. This system provides data on particle velocity and turbulent fluctuations. By seeding the flow with a low loading of very small particles that do move like the gas, velocity and turbulence characteristics of the gas may be obtained as well.

Optical techniques developed previously (Hayashi and Branch[1]) are used for measurement of particle concentration and for flow visualization. Particle concentration is measured by recording scattered light from a thin sheet of light focused through the centerline of the jet and by interpretation of the photographic record with an integrating densitometer (Figure 1). Conventional laser schlieren systems will be used for visualization of the shock wave location and structure in the jets (Figure 2).

Particle sampling probes are used to extract particles from the flow. The samples are then analyzed by a scanning electron microscope and a Coulter counter for measurement of size distribution.

Finite difference computer codes for nozzle and jet flow under development at Aeronautical Research Associates of Princeton seem best suited for comparison to our experimental results. The Standardized Performance Program (SPP) is used for nozzle flow correlations and the Standardized Plume Flow (SPF) code is under development for jet calculations including particle/shock interactions. Both are being supplied for use in the project.

Recent Publications

1. K. Hayashi and M.C. Branch, "Concentration, Velocity and Particle Size Measurements in Gas-Solid Two-Phase Jets," J. of Energy, 4, 193-198, 1980.

2. K. Hayashi and M.C. Branch, "Oblique Shock Waves in Two Phase Flow," Eighth International Colloquium on Gasdynamics of Explosions and Reactive Systems, Minsk, USSR, August 23-26, 1981; also Progress in Aeronautics and Astronautics, in press.

3. K. Hayashi and M.C. Branch, "Particle Transport Effects in Gas-Solid Two-Phase Nozzle and Jet Flow," Paper No. 81-2100, AIAA 14th Fluid and Plasma Dynamics Conference, Palo Alto, CA, June 23-25, 1981.

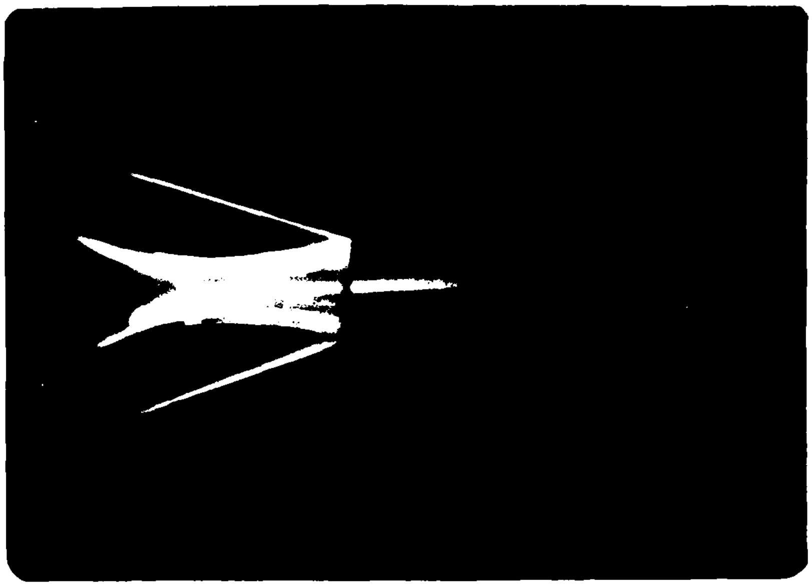

Figure 1. Flow visualization of particles concentrated along the centerline of a round jet moving from left to right out of a flow nozzle. The particles are concentrated along the axis because of their greater momentum. The gas surrounding the particles is accelerated in the nozzle and generally travels faster than the particles. Mechanical Engineering Combustion Laboratory Photograph.

Figure 2. A laser schlieren photograph of shock waves in a very high speed round jet. The pressure waves include oblique and curved shock waves due to the particles which can be seen in the center of the flow. Without particles the oblique shock waves are at a different angle and the curved shock waves are straight. Mechanical Engineering Combustion Laboratory Photograph.

COMBUSTION KINETICS OF METAL OXIDE AND HALIDE RADICALS AND METAL ATOMS

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Kinetic data, over wide temperature ranges, on combustion reactions of metal atoms, Me, and metal monoxide and monohalides, MeX, are essential input information for several aspects of Air Force Rocket Propulsion development. These include: air breathing propulsion, retarding or prevention of submicron metal oxide particle formation and advanced solid propellant formulations. To provide a means for establishing mechanisms and measuring rate coefficients and their temperature dependences, k(T), the HTFFR (high-temperature fast-flow reactor) technique was developed. This unique tool provides measurements on isolated elementary reactions in a heat bath. With traditional high temperature techniques such isolation is usually impossible to achieve; as a result, data on any given reaction depend on the knowledge of other reactions occurring simultaneously, leading to large uncertainties. HTFFR has primarily been used for the study of Me-oxidation reactions. In this recently initiated program, which includes some metal atom work, the emphasis is on providing similar data for MeX-oxidation reactions.

Figure 1 illustrates a modular HTFFR and its operation. The source section can include, e.g., a nonreactive vaporizer (used for Me reactions)[1], a high temperature gas/solid reaction source (under construction for BCl), or be replaced with a preparative flow line for MeX production (employed in the recent 300 K study of $BO + O_2 \rightarrow BO_2 + O$).[2] Figure 2 shows the type of 300-1900 K results which have been obtained for Me reactions, and which may be anticipated to result from the present program for MeX and Me reactions. It demonstrates the necessity to experimentally determine rate coefficients over wide temperature ranges, as clearly neither reaction obeys the simple Arrhenius law $k(T) = AT^{1/2} \exp(-E_A/RT)$, often assumed when extrapolating rate data obtained over narrow temperature ranges. The figure illustrates merely two types of non-Arrhenius behaviour; an extensive discussion of k(T) vs. T behaviour of combustion reactions, and our current understanding of it, is in preparation.[3]

The HTFFR being constructed for this program is of similar design to our earlier modular reactor, but the substitution of Pt/Rh resistance wire by SiC and Kanthal elements should lead to simpler maintenance and reduces costs. Its operation will be partially automated. Simultaneously we are working on BCl production methods, preparatory for a study of the BCl/O_2 reaction.

1. A. Fontijn, S.C. Kurzius and J.J. Houghton, Fourteenth Symposium (International) on Combustion, p. 167.

2. I.P. Llewellyn, A. Fontijn and M.A.A. Clyne, Chem. Phys. Lett. (in press).

3. M.A.A. Clyne and A. Fontijn, Eds., Reactions of Small Transient Species: Kinetics and Energetics, Academic Press, London (late 1982 or early 1983), Chaps. 1 and 2.

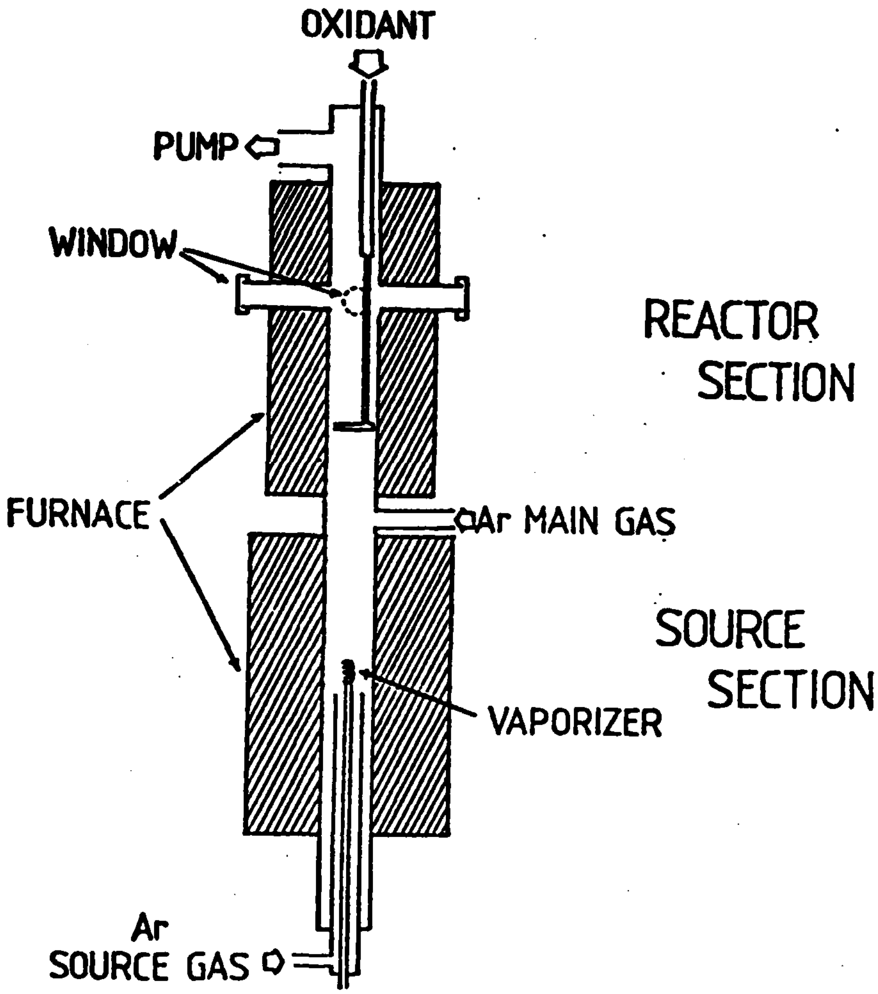

FIGURE 1: SCHEMATIC OF HTFFR APPARATUS FOR MEASUREMENT OF METAL COMBUSTION RATE COEFFICIENTS OVER LARGE TEMPERATURE RANGES.

- Reactant concentrations, pressure, temperature and average gas velocity are independently variable.
- Distance movable oxidant inlet to window plane is proportional to time.
- Measurement of MeX or Me concentrations is made at the window plane with a laser or hollow cathode lamp, respectively.

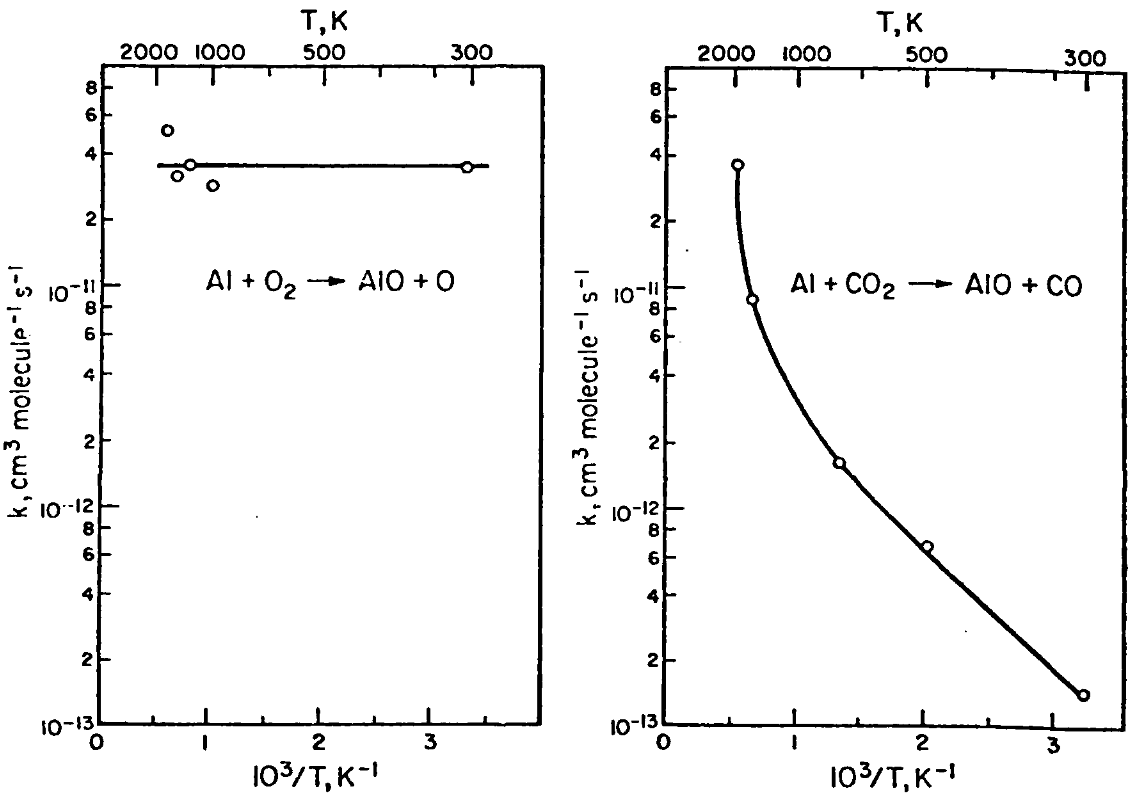

FIGURE 2: ARRHENIUS PLOTS OF THE Al + O_2 AND Al + CO_2 REACTION RATE COEFFICIENTS GROUPED BY TEMPERATURE.

Number of measurements at each temperature varies. The solid lines show the best fit to all data.

BEHAVIOR OF ALUMINUM IN
COMBUSTION OF SOLID ROCKET PROPELLANTS

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Robert K. Sigman

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Atlanta, Georgia 30332

The general objective of the present research is to understand and control the complex sequence of behavior of the powdered aluminum ingredient of solid propellants during propellant combustion. The general nature of the processes governing concentration of aluminum on the burning surface, ignition and coalescence into burning agglomerates, has been established by past work on this and other projects, as has the subsequent burning history and formation of oxide droplets. However, there are certain key steps that are either controversial, or not understood well enough to predict or control combustion behavior or extrapolate to all propellant systems (Fig. 1). Current work is directed at those questions, which are noted below, and which will be discussed in the presentation.

1. What microstructural details of the heterogeneous propellant and aluminum particles are conducive to concentrations of particles on the burning surface (studied primarily by observing effects of changes in propellant microstructure).

2. What processes restrain particles on the burning surface and concentrate them to a state necessary for coalescence (studied by observing effects of changing the binder, changing the oxide in the aluminum, and observing sintering behavior of aluminum powders in controlled tests).

3. What are the combustion zone conditions that lead to inflamation of accumulations of aluminum (photographic observation of inflamation; inference from quenched samples; inference from effect of manipulation of flame conditions by test sample microstructure).

4. What governs the burning rate of oxide-lobed agglomerates in propellant combustion environments (studied by analysis of particles quenched from the combustion plume).

5. What is the nature of the terminal phase of agglomerate burning, when the oxide lobe dominates the droplet. Does fragmentation occur? (Studied by examination of quenched particles and populations).

6. What portion of the oxide products is in the form of residuals from oxide lobes (as compared to smoke), and what is the size distribution (studied by plume quenching and analysis of particle population).

One of the more significant results follows from two earlier observations.

1. Accumulated aluminum is ignited by the high temperature oxidizer-binder flame.

2. In bimodal oxidizer propellants, the finer oxidizer particles fail to establish a high temperature flame because the environment is locally fuel rich.

The result of these two observations is that aluminum in propellants with bimodal oxidizer accumulates and agglomerates much as if no fine oxidizer were present. Agglomeration is minimized by increasing the size of the fine oxidizer until dispersal of the aluminum in the microstructure is maximized. (Fig. 2)

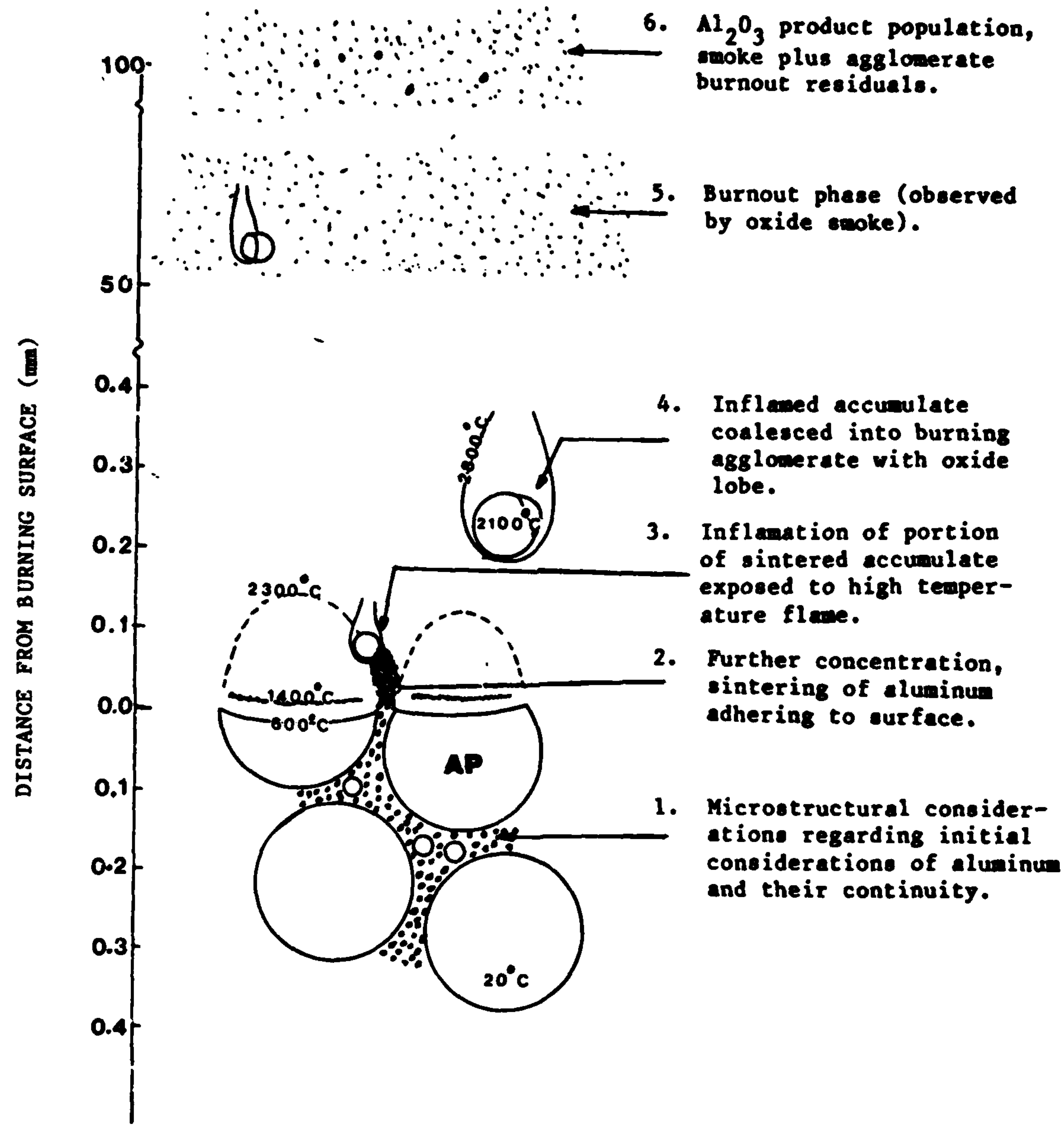
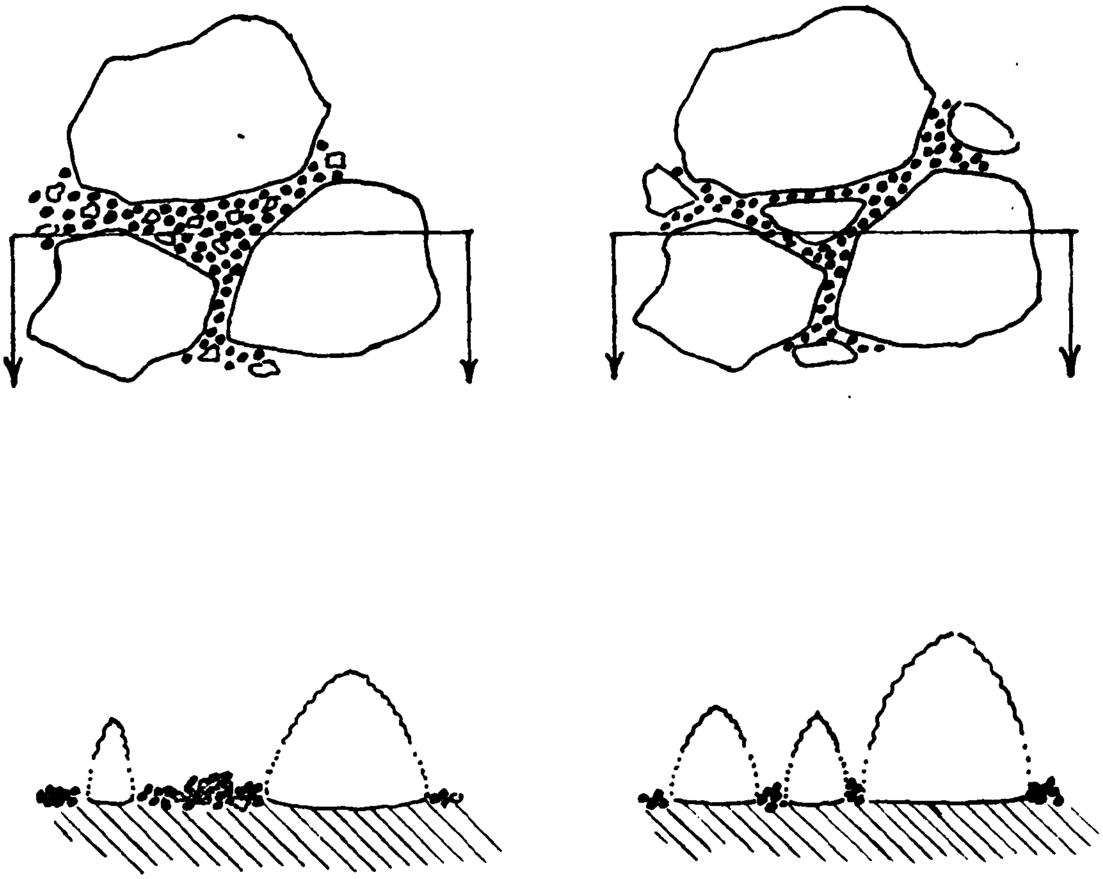


Fig. 1 Critical processes in agglomerate formation in combustion.



BIMODAL AP
COARSE & FINE

Large areas of fine AP and aluminum, AP too fine to establish local diffusion flames and aluminum ignition.

LARGE AGGLOMERATES

BIMODAL AP
COARSE & INTERMEDIATE

"Fine" AP is coarse enough to disperse aluminum, and provide additional local diffusion flamelets to ignite aluminum.

SMALL AGGLOMERATES

Fig. 2 Sketches illustrating how oxidizer particle size affects dispersion of aluminum and proximity to ignition sites on the burning surface.

DETERMINATION OF THE COMBUSTION MECHANISMS OF ALUMINIZED PROPELLANTS

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Composite solid propellants containing powdered metals are of interest due to their highly energetic and stable combustion characteristics. However, prediction of the performance of a solid rocket motor is difficult if it burns metalized solid propellants. This is primarily due to the unknown factors associated with metal particle/agglomerate two-phase flow behavior within the motor combustion chamber and nozzle. A thorough investigation is being conducted for determining important mechanisms associated with metal combustion including those controlling surface/near surface agglomeration, metal particle/agglomerate combustion characteristics in a motor environment, and particle breakup and two-phase flow behavior in a nozzle flow field.

This experimental research program involves measuring the aluminum/aluminum oxide particle size and size distribution under carefully controlled conditions simulating the combustion chamber and nozzle entrance region of a solid propellant rocket motor. The major emphasis of this past year has been in the construction and check out of a servo-positioning strand window bomb. This laboratory scale combustion device has been demonstrated to be capable of burning strands of solid propellant under high pressure conditions while holding the burning surface fixed in space to an accuracy of approximately plus or minus 100 microns, or close to the scale of the surface roughness. Better spatial resolution is expected as experience with the servo-positioning system is gained. While the propellant strands are burning within the bomb, a computer controlled data acquisition system extracts instantaneous burning rate and environmental condition data for analysis.

With the servo-positioning strand window bomb capable of holding a burning propellant surface stationary in space, aluminum/aluminum oxide particle size and size distribution data can then be extracted by means of an existing imaging-type particle size analyzer. This device consists of a pulsed light source, a Motorola closed circuit television camera as an imaging receiver, the Purdue/Parker Hannifin electronic package to decipher and analyze the data, and a PDP 11VO3 computer to process the data. Such an imaging-type particle size analyzer is unique in that it should prove to be an accurate, non-intrusive diagnostic tool for particle size and size distribution measurements within simulated motor chamber/nozzle flowfields. At the present time, additional motor chamber/nozzle flowfield simulating devices are being designed and fabricated to be used in place of the servo-positioning combustion bomb in order to investigate aluminum/aluminum oxide particle behavior.

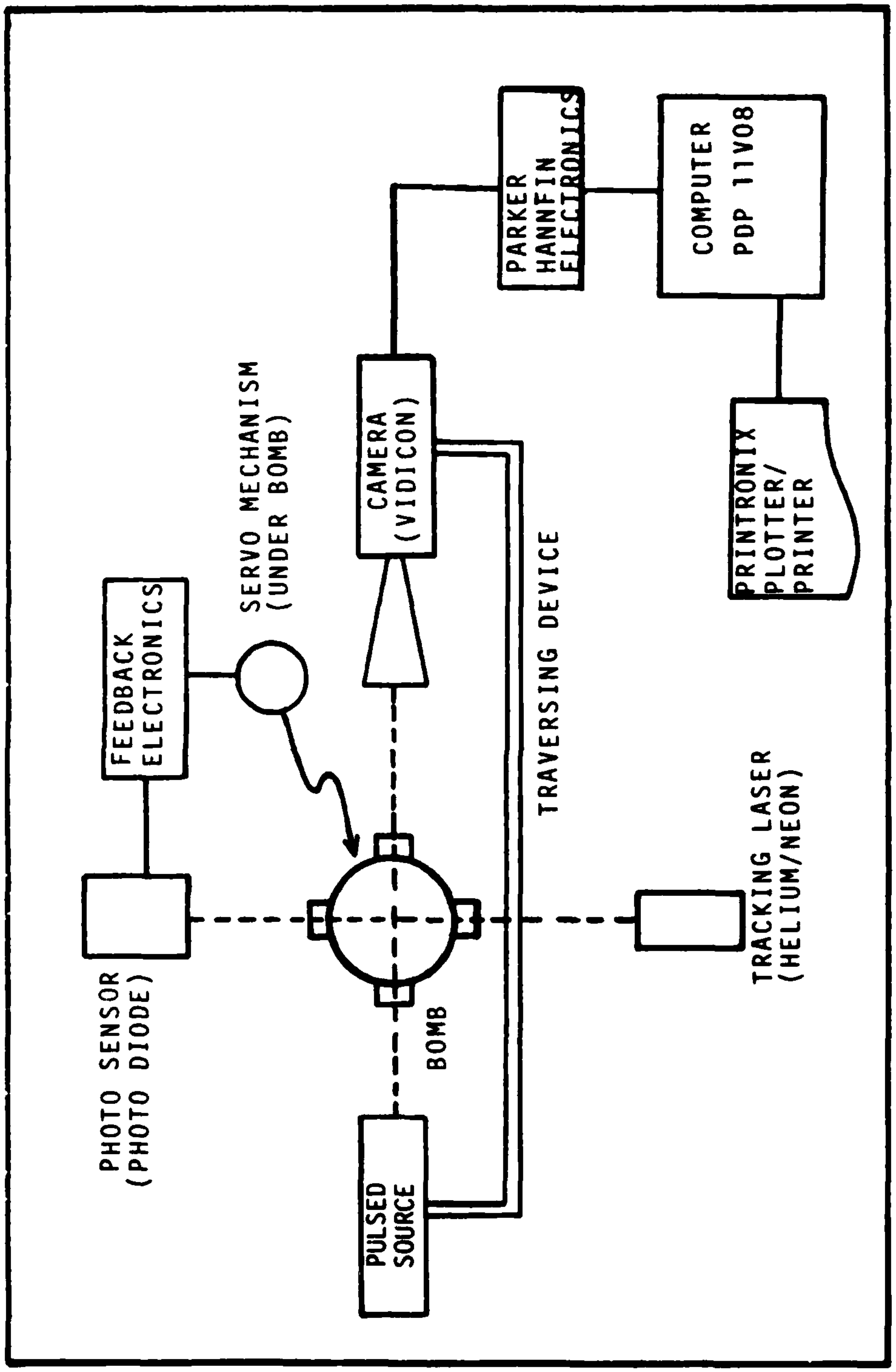
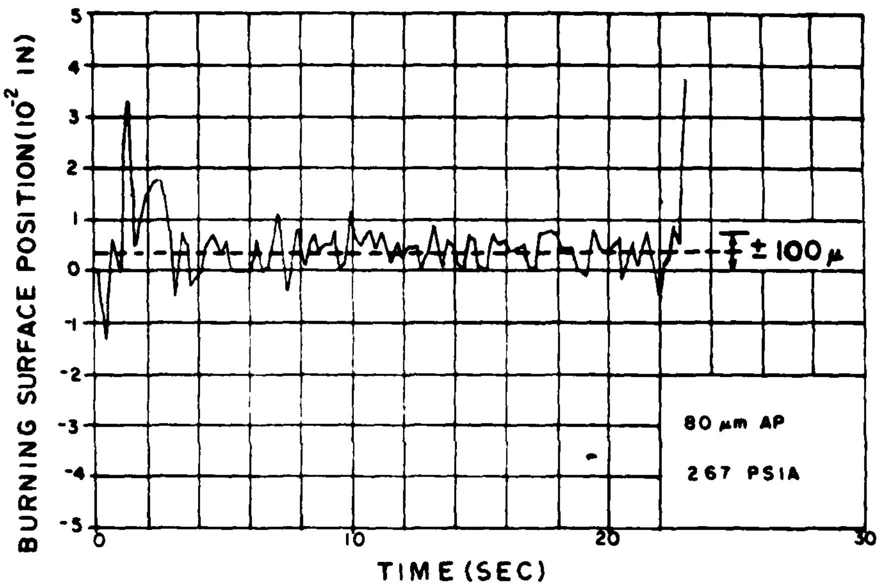
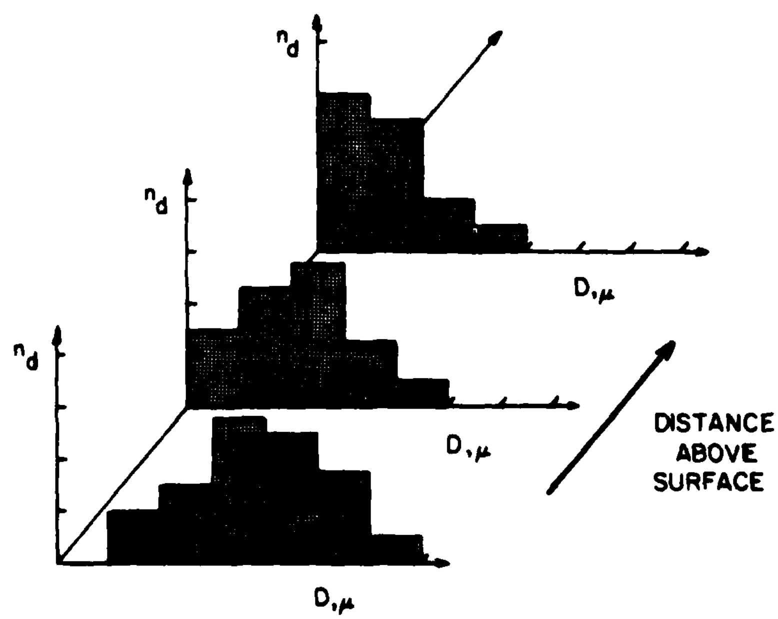


DIAGRAM OF EXPERIMENTAL APPARATUS

FIGURE 1



Experimental: Sample Burning Surface Position Response.



Experimental: Expected Size Distribution Results.

FIGURE 2

ABSTRACT

AERODYNAMIC DROPLET BREAKUP

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The breakup of Al/Al_2O_3 agglomerates associated with aluminized propellants appears to be an important process in determining particle size distribution and two phase flow effects on combustion efficiency in solid rocket motors. While direct observation of agglomerate breakup has been made under realistic flow conditions, the basic mechanisms involved have not been defined or characterized. The basic mechanisms of agglomerate breakup may differ significantly from those associated with the breakup of water droplets and other liquids with more conventional physical properties. The present investigation is directed toward an improved understanding of the fundamental mechanisms of droplet breakup with particular emphasis on high surface tension liquid droplets within nozzle flow environments.

This abstract describes the first year's efforts to investigate aerodynamic breakup of conventional liquid droplets (Figure 1). Water, freon, and glycerine were selected to enable variation of surface tension and viscosity. A two-dimensional aerodynamic nozzle was configured to subject injected droplets to an aerodynamic load sufficient that droplet breakup would occur within the nozzle contraction. Ink jet droplet generators were used to produce highly monodisperse droplets ranging in diameter from 50 to 800 μm. The droplet Weber number, a measure of the ratio of aerodynamic deforming forces to surface tension restoring forces, was established by preselecting droplet size, droplet liquid, and gas velocity. Pulsed laser holography was used to observe the breakup of liquid droplets. The holocamera trigger beam was scanned along the droplet stream to observe the droplet breakup process.

The breakup of freon droplets (800 μm diameter), a relatively low surface tension liquid, is depicted in Figure 2. Two phases of the breakup process are evident: the initial in which the droplet is deformed and the final in which the droplet fragments. During the initial phase, the droplets flatten. Then a branch appears to form and grow from the downstream side of the droplet carrying liquid away from the main body. The branch will eventually detach from the main body in a process which forms a cloud of smaller droplets. However, sometimes, and more randomly, smaller branches will form and detach from the primary branch before the larger branch can detach. The smaller droplets are quickly accelerated away from the main body which continues to feed fragments into the flow. Preliminary results indicate that the size of the droplet fragements is about 10 percent of the initial droplet diameter and that fragment size decreases with increasing Weber number.

Droplet breakup experiments are underway in which freon, water, and glycerine droplets from 50 to 250 μm diameter are observed in Weber number conditions of 30, 60, and 90. Data analysis will include a discussion of the effect of surface tension or Weber number and viscosity on the breakup mechanism, time scale, and on the resultant fragment size distribution. Droplet breakup experiments will also be attempted with a two phase liquid slurry composed of neutrally buoyant spheres dispersed within a water droplet. The second year's effort will concentrate on higher surface tension metallic liquids which more closely simulate the liquid properties of aluminum. Much of the current technical approach will be utilized including aerodynamic acceleration, ink jet generation, and holographic observation.

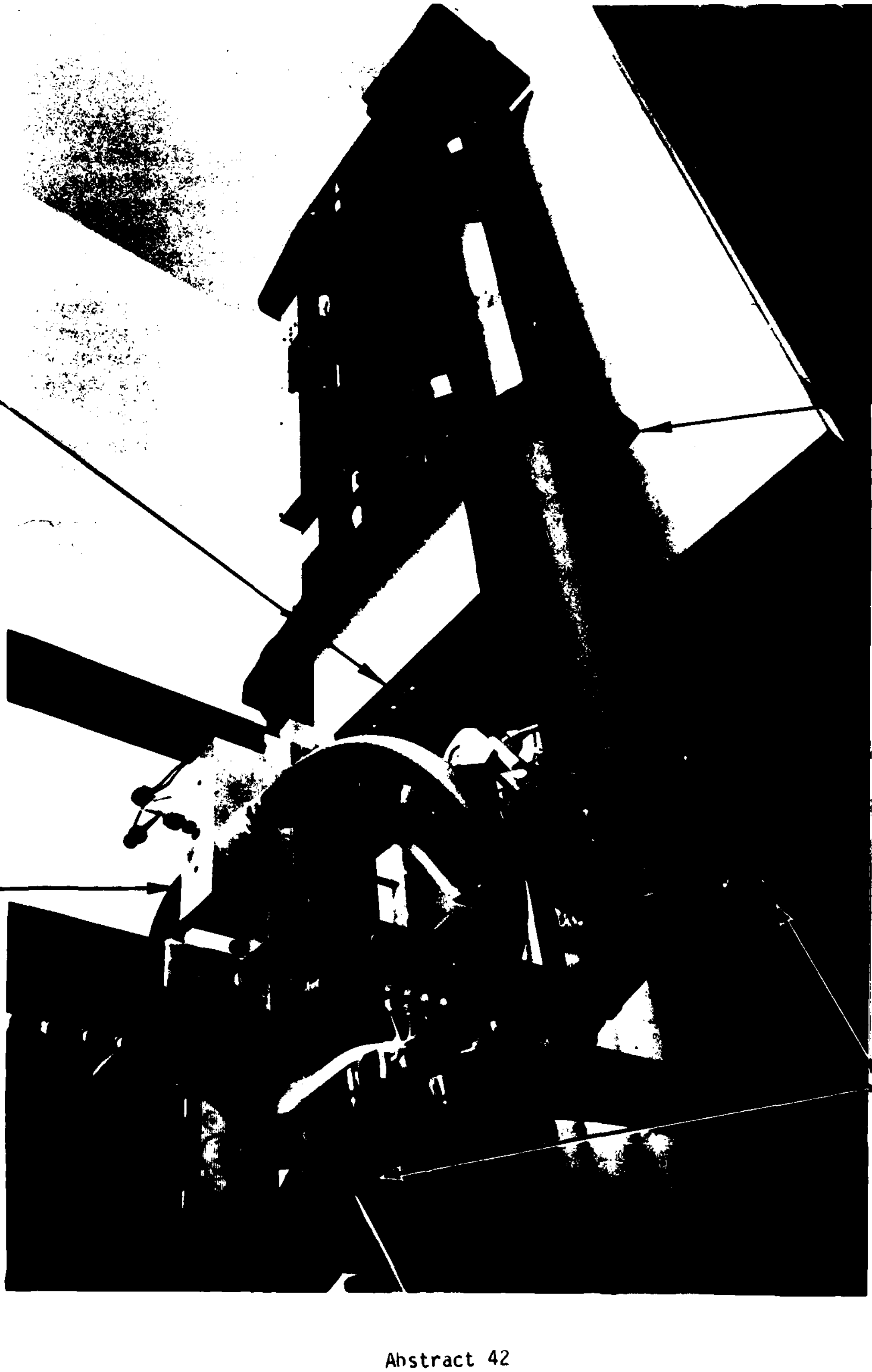

FIGURE 1. AERODYNAMIC DROPLET BREAKUP EXPERIMENT

AERODYNAMIC DROPLET BREAKUP

Weber Number 90• 60m/s Velocity
800μm Freon Droplet

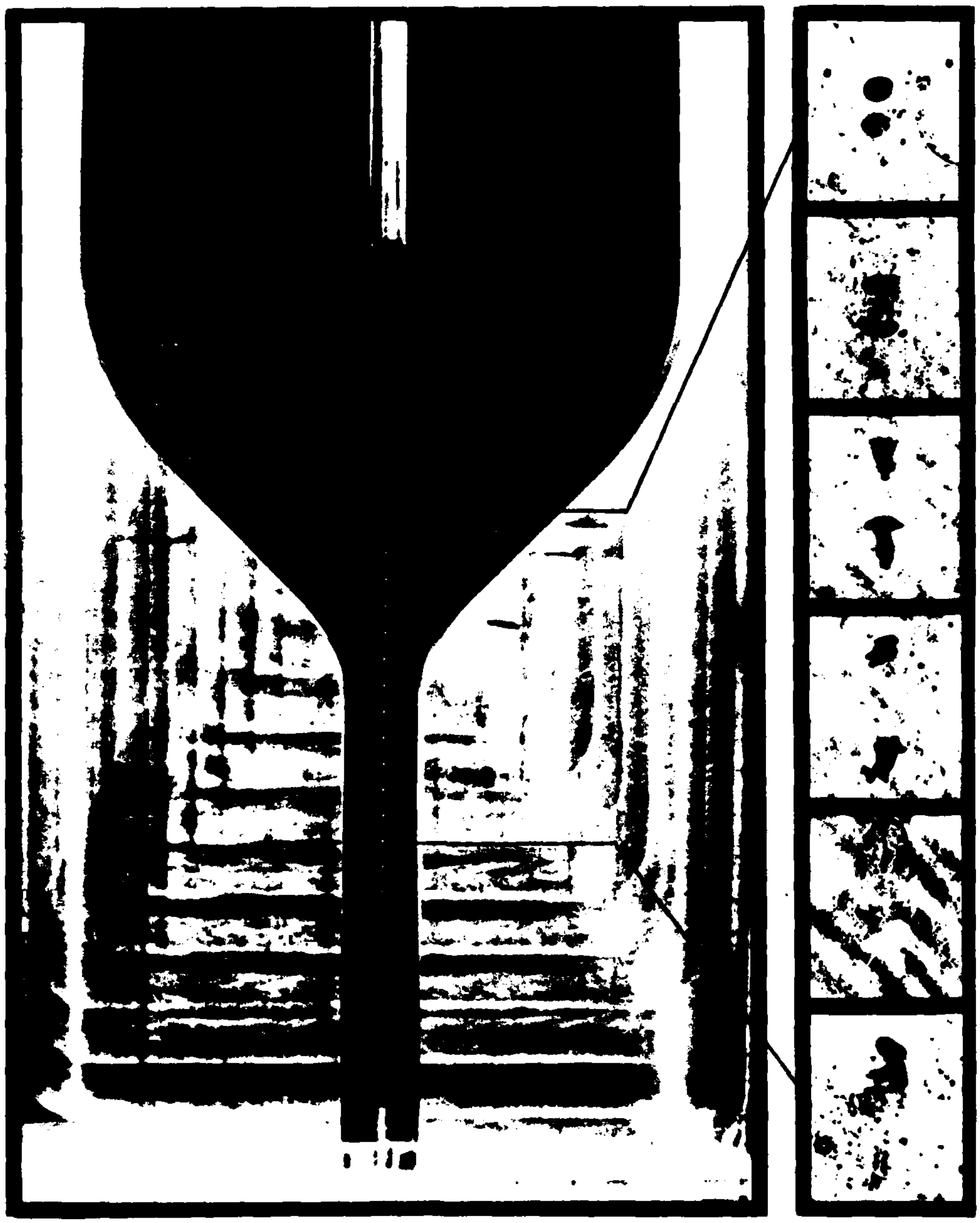

FIGURE 2. FLASH PHOTOGRAPH OF MONODISPERSE DROPLET GENERATION IN QUIESCENT AIR AND DOUBLE PULSE ($\Delta\tau$ = 400 μs) HOLOGRAPHIC RECONSTRUCTION OF DROPLET BREAKUP PROCESS ALONG THE AERODYNAMIC NOZZLE.

EFFECT OF ACCELERATION ON METALIZED COMPOSITE PROPELLANTS

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The research will enable the specific impulse trends to be predicted as a function of formulation variables and operating conditions for low-spin stabilized solid rocket motors. An understanding of the mechanisms of metal combustion, agglomeration, and breakup as they relate to gas flow environments representative of chamber conditions are sought. Both experimental and analytical approaches are employed. Surface agglomeration is observed using high-speed films from AFRPL'S Spin Window Bomb. Observations from these experiments, coupled with first principle modeling are being incorporated in the Aluminized Petite Ensemble Model. Improved experimental techniques in propellant photography are currently being analyzed and tested to provide more precise data. Molten metal particle behavior in accelerating flow fields will be studied in a shock tube device at Purdue University. This method incorporates a unique acoustic particle holder, laser particle igniter, and high-speed photography. Control of gas properties, with measurements of particle trajectory and breakup will lead to substantion or improvement of agglomerate breakup criterion and provide basic data for the prediction of trajectory burning particles. Work completed on surface agglomeration includes observations of SWB films, development of data reduction programs, first generation agglomeration modeling, and exploratory photographic studies. In the particle breakup investigation, a review of literature, shock tube design and hardware acquisition, acoustic pressure analysis, and laser ignition specifications, have all been completed. Future work will extend the above efforts with an emphasis on incorporating the data obtained into mathematical models.

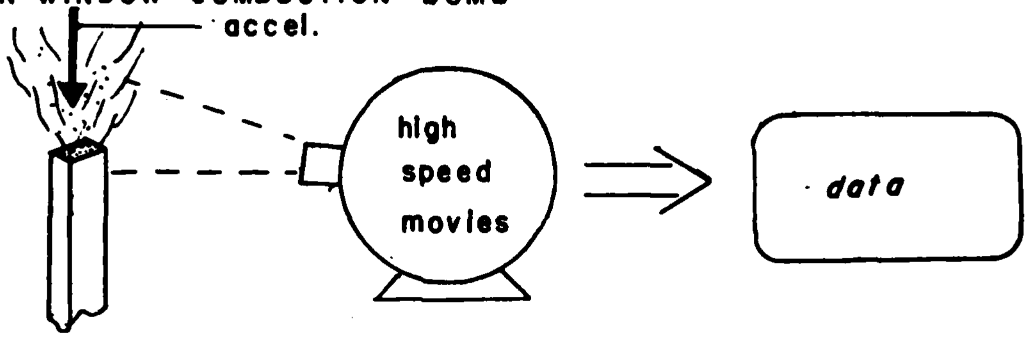
SCIENTIFIC APPROACH

1. HYPOTHESIZE BEHAVIOR WITH BASIC PRINCIPLES

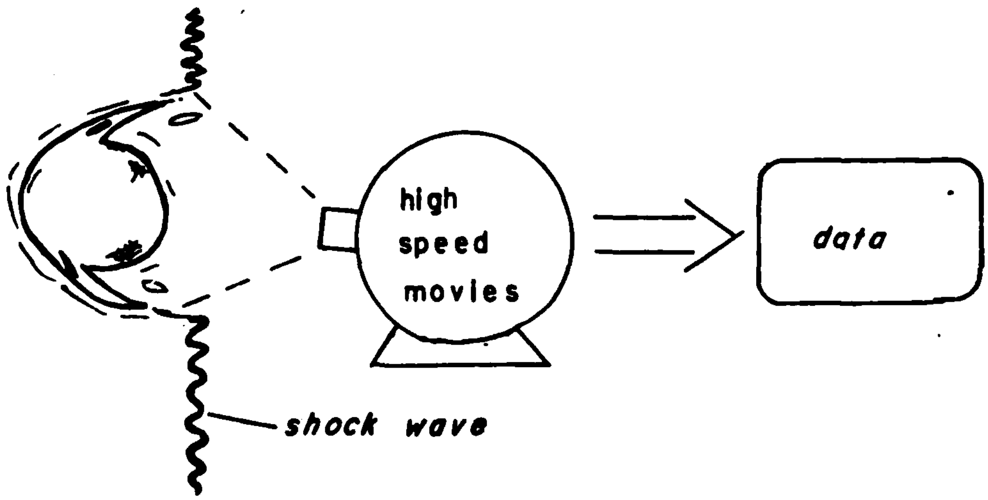
- PROPELLANT COMBUSTION THEORY
- PARTICLE BREAKUP THEORIES
- INTERNAL BALLISTICS

2. SMALL SCALE EXPERIMENTAL TESTING

- SPIN WINDOW COMBUSTION BOMB



- PARTICLE BREAKUP SHOCK TUBE



3. COUPLING OF HYPOTHESIZED PRINCIPLES WITH DATA

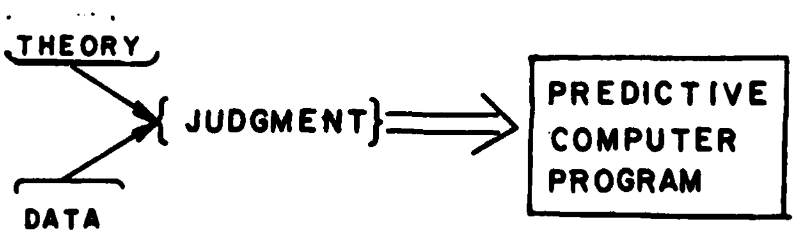


FIGURE I

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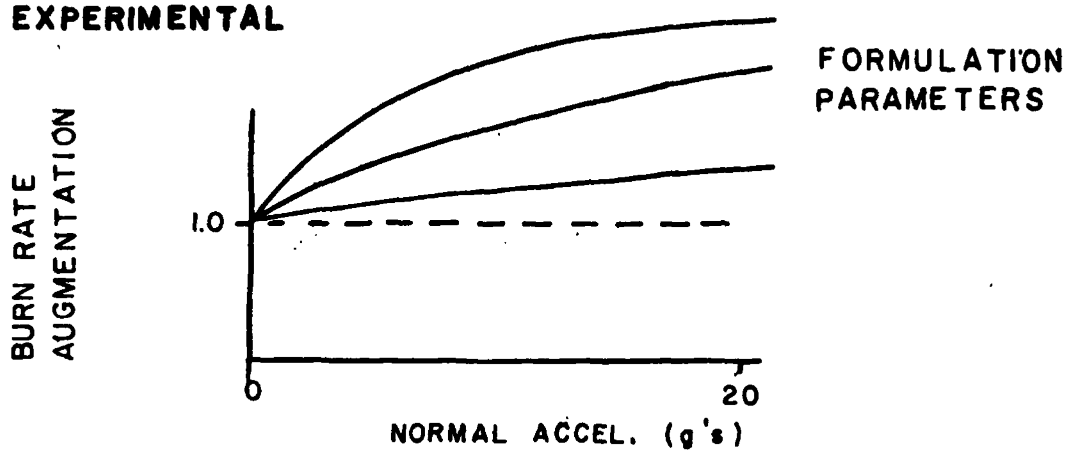
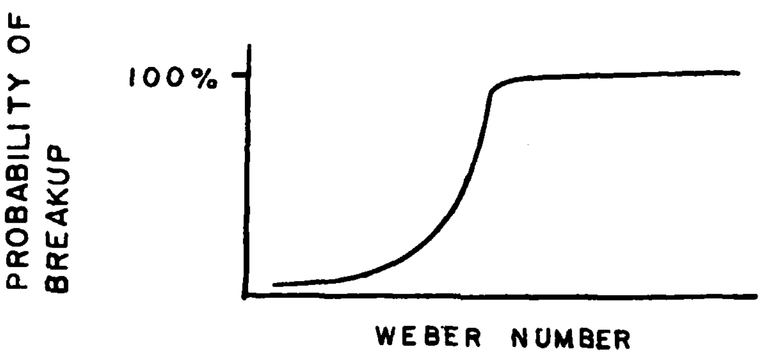
ANTICIPATED RESULTS

1. EXPERIMENTAL





2. COUPLED

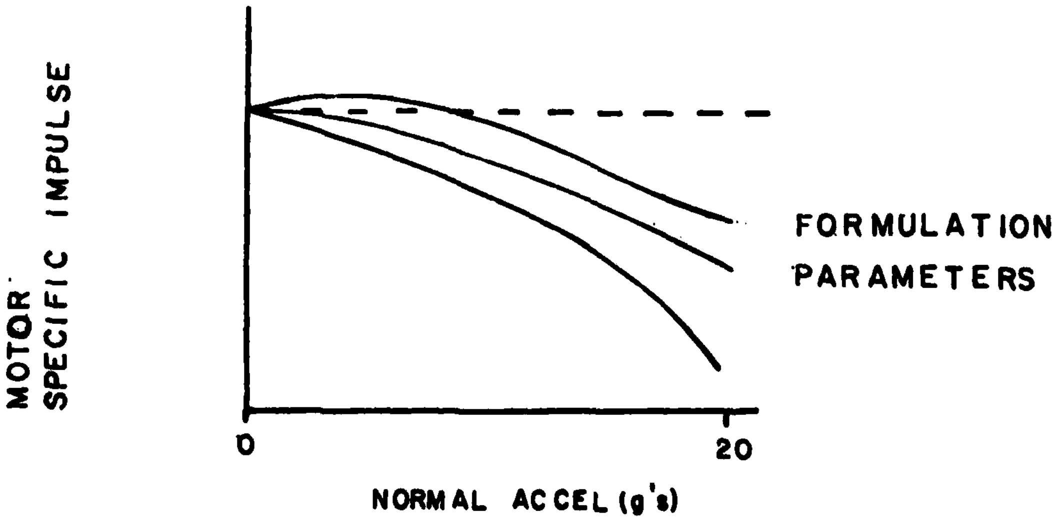


FIGURE 2
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APPENDIX 1

DIAGNOSTICS IN REACTING MEDIA

Approach

In FY81, an multidisciplinary research task was begun to provide new diagnostic techniques which are needed for the advancement and understanding of combustion systems, air-breathing and rocket engines, efficient fuel utilization, plume signatures, and signal attenuation. This task is parallel to the present tasks on rocket propulsion and air-breathing propulsion. The research is helping to overcome defficiencies in obtaining reliable measurements of important parameters in the reacting flows of practical, hostile combustion environments and the inability to reliably evaluate combustion models. The research objectives include: to originate more sensitive, selective, precise, reliable, and rapid diagnostic methods for measuring important parameters in air-breathing and rocket engine reacting flows; to investigate, validate and apply the instrumentation concepts; and to measure fundamental parameters required to implement the approaches. The results will aid in reducing to practice new in-situ nondisturbing techniques for accurately measuring reacting flows. While many of the physical principles have been anticipated, this endeavor will enable combustion researchers to confront the realities of obtaining useful measurements. Investigation, verification and application of advanced instrumentation and diagnostics for reacting flows is being conducted as an integrated, multidisciplinary program. For example, combustion scientists have identified measurement needs and interacted with physicists, chemists, et al to incorporate advances in areas such as optics, molecular dynamics, and sensors. Physical phenomena which have promise for new diagnostic techniques are being explored. Where necessary, fundamental physical parameters needed to implement the techniques will be determined. Techniques will be validated through intercomparisons with standard techniques and laboratory scale reacting flows.

Specific Goals:

Noninterfering Diagnostic Techniques - To explore the application of diagnostic techniques that do not disturb flow conditions for measuring the gas and gas/particle flow properties representative of rocket systems including plumes. To improve understanding of the factors involved in sensing and detecting the chemical and physical properties related to rocket flow systems. To determine the advantages of each technique and define their respective zones of applicability for propulsion systems.

Kinetics of Multicomponent Condensation - To achieve methods of performing quantitative measurements for gas/particle systems so that the influence of composition and flow environment on particle formation and growth characteristics and range of particle sizes can be investigated.

Energy Exchange Rates - To improve the methodology for measuring species concentrations in exhaust plumes so that emission and absorption contributions associated with nonequilibrium processes can be isolated.

Chemical Kinetics for Nozzle and Plume Flows - To improve and devise methodology for determining the spatial and temporal distribution of important species so that rate processes can be measured. Attention is to be given to multi-dimensional flows.

Combustion - To explore methods for obtaining rate data for solid and liquid energetic materials being heated at ratios in excess of 10^3K/sec.

Combustion Instability - To investigate methodologies for measuring the unsteady velocity, pressure, and temperature components in multi-dimensional unsteady reacting flows. Particular emphasis is to be given to acoustic level excitations and responses. To visualize nonsteady, multi-phase flow and condensed phase breakup for the purpose of understanding the role of transient processes on acoustic energy gains or losses.

Metal Combustion - To improve methods for simultaneously measuring temperature and concentration of turbulent flame zones of multi-phase media so that conditions leading to metal combustion under ram-rocket conditions (particularly high altitude) can be characterized.

Status

Instrumentation and Diagnostics - Both tunable dye and diode laser absorption spectroscopy are being extended to include additional species, optical probes, time dependent flows and particle-laden flows. The understanding of CARS processes is being improved with respect to conversion efficiencies, line shape, and turbulence effects (via cw and pulsed measurements). With respect to tomography, techniques for fast scanning and recording multidetectors are being investigated along with improved deconvolution schemes. Fiber optics used in conjunction with several diagnostic methods are being explored as means of probing hostile flows. Quantitative flow visualization (species concentration, velocity and temperature) are being explored using laser illumination of planar regions. As tests of technique suitability the following physical situations will be investigated: turbulent reacting, shear layer flow to understand the coupling between fluid dynamic and chemical processes; droplet evaporation in turbulent flows; flows with high particle loadings. The applicability of absorption-emission techniques as 3-D combustion diagnostics is being investigated. Using multiangular scanning, sequential layer methods are being extended from axisymmetrical flows to arbitrary distributions of species in reacting flows encountered in actual 3-D combustion systems. The concept of an emission technique based on the instantaneous measurement of multiple fans from several windows is being evaluated which can provide an instantaneous map of temperature and species concentration. Specific emphasis will be on tomography of particulates of arbitrary size distribution. Specific emphasis is being placed on determination of the capabilities and limitations of the vibrational Raman scattering (VRS) as a laboratory diagnostic tool. The potential of resonant CARS is being explored to establish the optimum input frequencies and to search for double frequencies to enhance detectivity.

Kinetics of Multicomponent Condensation - A research program is being directed at quantitative data interpretation techniques for visualization of multi-phase flow, condensed phase breakup condensation, and particle growth. The approaches being considered include multi-pulse holographics and the determination of particle size distributions and velocities from multipulsed holograms.

Energy Exchange Ratios - Pico second excitiation techniques are being explored to establish the potential of photon echo signals to provide information on molecular transport phenomena. Initially data will be obtained that relate to quenching and rotational relaxation rates for OH in flames.

Chemical Kinetics for Nozzle and Plume Flow - Fiber optics probes are being evaluated for use in conjunction with several of the optical diagnostic methods. The goals are to hardened remote units and to provide moveable probes which can transmit signals and optical beams to and from the experiments and full scale combustors.

Combustion - A research program is contemplated that will consider techniques for rapidly following the temperature increases, compositional changes, and phase changes that occur within a rapidly decomposing or burning energetic material. The possibilities include optical tracking of crystaline transformation and acoustic frequency changes related to bulk temperature.

Combustion Instability - An approach for remotely measuring velocity components in reacting flows is based on simultaneously measuring conductivity and the conductivity-velocity product. Analyses indicate that using multi-coils, based on magnetic dipole primary induction field, the conductivity and the flow velocity vector components can be calculated directly from secondary coil voltage measurements. Simulation calculations and bench top experiments are now in progress.

Metal Combustion - In-situ measurements of particle size distribution is being undertaken of using two-wavelength transmissometry, forward Mie scattering and wire filter probes.

This broad area includes opportuinties for new research, e. g.,

1) Ultra-high speed reaction detection of the kinetics of crystal phase change and liquid layer decomposition of energetic materials.

2) Quantitative measurements in reacting two phase flows, e.g. 2-D concentrations, temperatures, velocities of both phases, 2-D mixing parameters at shear flow interfaces.

APPENDIX 2

OVERVIEW OF ROCKET PROPULSION RESEARCH GOALS

General Objectives
Research in support of rocket propulsion is directed at improving performance and toward developing a scientific understanding of phenomena associated with the generation of propulsive power through energy conversion processes which are primarily self-contained. Research is needed from molecular to macroscopic scale in areas which include the dynamics of rocket combustion, the behavior and synthesis of propellant and nozzle materials, the characteristics of exhaust plume formation and radiation, and the dynamics of electromagnetic propulsion. Further knowledge is needed in these areas to meet mid-term and long-term Air Force technology goals related to improving performance, reliability, penetrability, and durability for Air Force mission applications involving ballistic missiles, air launched missiles and propulsion in space. However, specific provisions are also included for research directed toward scientific opportunities which cannot be related to particular mission areas at this time.

Specific Goals
The following paragraphs summarize many of the current goals, many of which are the subjects of ongong research.

Solid Mechanics - To improve understanding of damage tolerant design for new materials through extensive empirical and analytical approaches. Investigate fatigue, damage propagation and detection, fracture, and effects of spectrum loading and sequencing. Extend the existing theories to three dimensions, including the interaction between viscoelastic behavior and damage, the micromechanics of propellant structure, and the effects of temperature to obtain a theory that will predict propellant stress-strain behavior from simple tests. Establish an age-life model based on chemical reactions.

Noninterfering Diagnostic Techniques - To achieve improved diagnostic techniques for measuring the gas and gas-particle flow properties representative of rocket systems including plumes. To improve understanding of the factors involved in sensing and detecting the chemical and physical properties related to rocket flow systems. To devise and improve diagnostic techniques to obtain rapid and quantitative spatially and temporally resolved measurements of temperature; pressure; velocity; species concentrations and densities; and particle/droplet size and distribution in optically dense, high-temperature reacting, unsteady, turbulent flowing media, including combustors and exhaust plumes. To determine the advantages of each technique and to define their respective zones of applicability.

Kinetics of Multicomponent Condensation - To achieve methods of performing screening measurements for gas/particle systems so that the influence of composition and flow environment on particle formation and growth characteristics and range of particle sizes can be investigated. To characterize and obtain numerical data on the condensation processes occurring in pure and mixed flows. Available predictive models for nucleation and condensation in multi-component, multiphase systems are to be verified and improved.

Formation Mechanisms/Chemistry of Metal Oxide Particles - To characterize the basic mechanisms and chemistry involved in the formation of metal oxide particulates. To experimentally determine the physical and chemical processes of metal droplet combustion. To explore methods of greatly reducing the size of metal oxide agglomerates entering nozzle convergent sections.

Chemical Kinetics for Nozzle and Plume Flows - To determine reaction pathways and to obtain rate data for combustion chamber, nozzle, and exhaust plume flows. To improve and devise methodology for determining the spatial and temporal distribution of important species so that rate processes can be measured. To determine the reactions and mechanisms occurring at the surface of solid rocket propellants. To study detailed kinetic processes of light diatomic and triatomic free radical species important in combustion chemistry.

Solid Propellants - To discover higher energy materials suitable for solid propellant formulations. To determine the behavior of nitramine (e.g., HMX and RDX) composite propellants during combustion and to characterize mechanisms which may lead to detonation. To establish relationships between molecular structure and decomposition processes.

Synthesis of Propulsion Materials - To synthesize tough, high energy elastomers having low glass-transition temperatures. To achieve a practical technique of synthesizing vinyl prepolymers having terminal functionality and to improve polymer characterization methods. To synthesize new propellant curatives, characterize migration rates of mobile ingredients, and improve techniques to determine polymer properties. To conduct original synthesis of new, energetic propellant ingredient materials.

Combustion - To understand important heat release mechanisms so that research to modify burning rate and combustion efficiency can be directed at specific reaction sites. To explore methods for obtaining rate data for solid and liquid energetic materials being heated at rates in excess of 10^4K/sec. To determine the effects of an acceleration-fields on propellant ballistics. To characterize the mechanisms leading to changes in solid propellant properties and burning modes that can lead from normal deflagration to detonation of rocket motor grains.

Combustion Instability - To improve analytical methods for predicting the stability behavior of solid motors through development of theories to treat mechanisms such as nozzle damping, acoustic erosivity, pressure coupling, velocity coupling, distributed combustion, particle and structural damping, and high velocity effects. To include effects of realistic geometries. To examine more direct means of measuring acoustic admittance. To extend the use of laser doppler velocimetry as a means of measuring steady and unsteady combustion characteristics of solid propellants. To investigate methodologies for measuring the unsteady velocity, pressure, and temperature components in multi-dimensional unsteady reacting flows. To visualize nonsteady, multi-phase flow and condensed-phase breakup for the purpose of understanding the role of transient processes on acoustic energy gains or losses. To focus attention on frequencies up to 40 kH. Causes and mechanisms of velocity coupled combustion instability (VCCI)

need to be determined and characterized in terms of flow field parameters. Data verification needs to be conducted for new combustion response measurement devices.

Metal Combustion - To improve methods for simultaneously measuring temperature and concentration of turbulent flame zones of multi-phase media so that conditions leading to metal combustion under ram-rocket conditions (particularly high altitude) can be characterized. To assess the role of fluorine in the combustion of fluorinated metallic propellants and to determine mechanisms that affect oxide particle size. To understand and to analytically describe the basic phenomena of metal particle combustion in solid and ramrockets. To quantify processes leading to formation of micrometer size oxide particles.

Thermophysical Properties - To increase the scope, usefulness and reliability of the JANAF Thermochemical Tables; to obtain needed measurements of thermodynamic properties of combustion products of metallized propellants; and to measure fundamental vibrational frequencies and other molecular constants for accurate calculation of ideal gas properties of high temperature species.

Surface Reaction Kinetics of Carbon/Carbon Composites - To establish the relationship between carbon/carbon material processing variables and the kinetics of reaction of these materials with gases representative of rocket exhausts.

Alternate Energy Sources for Propulsion - To achieve advanced propulsion concepts capable of pounds of thrust at several thousand seconds of specific impulse.

APPENDIX 3

SPACE POWER AND PROPULSION
- FY83 INITIATIVE -

GENERAL OBJECTIVE: Future Air Force space missions for communications, surveillance, and weapons systems will require substantially higher power and more efficient propulsion for orbit raising . Research is expected to lead to improvements of 20% in propulsion efficiency with improved liquid and solid propellants and 100 to 300% with non-conventional systems such as energy beaming, magnetoplasmadynamics, nuclear, and mass accelerators. At least, three-fold improvements in continuous power (megawatt) and energy density as well as ten-fold improvements for pulsed power and associated storage and conditioning subsystems are anticipated.

To contribute to achieving these, research initiatives will include the following basic studies: elimination of material degradation by corrosive higher energy oxidizers, prediction of low pressure combustion conditions for light metal fuels, categorization of toxicity, accurate models to predict the coupling of beamed energy sources to the working media, establishing small scale research experiments that are valid for understanding full size configurations, achieving compact heat rejection systems through new refrigeration and radiation concepts, fundamental studies to improve efficiencies of power systems, and basic investigations of nonconventional power sources.

STATUS: Orbit raising propulsion and space power (in particular megawatt or greater) are topics which periodically receive high level attention but only moderate follow-up basic research activity. However, the projections for the 1990's define the needs for sustained basic research activity. The space shuttle capability plus the inevitability of the dominate Air Force role in space are forcing definitions of major new propulsion and power requirements.

In the last three decades, a large number of important concepts have been recognized. Prior to the present considerations, the concepts could have been placed in several categories, e. g.,

1. Sufficient onboard power did not exist for specific propulsion concepts.
2. Air Force requirements did not justify further research.
3. Solutions to fatal flaws could not be foreseen.
4. Potential for space contamination was too great.
5. An important technology was lacking.
6. Knowledge of the concept was narrowly held, thus it escaped attention.
7. Performance penalties were too great.

But probably the dominate consideration in previous years was that the Air Force could perform the required missions with conventional approaches. Consequently, major initiatives to provide technology and to overcome specific barriers were not warranted. The projected missions coupled with the technical advances of the last decade prompt a revaluation of past judgements to establish new basic research directions.

3Dec81/0031G

SPECIFIC GOALS:

1. Power Generation - To improve the efficiencies and operational parameters of chemical and radiant power sources of tens of megawatts(electrical). To overcome the basic problems limiting the application of nonconventional ten- to hundred- megawatt(electrical) power sources, such as nuclear and beamed energy. To extend power density of closed-cycle energy conversion systems.

2. Thermal Management - To realize more weight efficient and less vulnerable heat rejection concepts, to lower the maximum rejection temperature, to provide concepts for higher thermal transmission rates and for pathways incorporating space station structures.

3. Power Distribution and Energy Storage - To reduce losses from power distribution and to extend range of operation, to increase energy storage density throught novel energy storage concepts.

4. Beamed Energy - To quantify mechanisms of energy transfer to working fluids, to assess the barriers to optical access for energy transmission, and to establish approaches for plasma confinement. To enable consideration of candidate energy beams with the most effective working fluids.

5. Electromagnetic Acceleration - To understand electromagnetic and magnetoplasmadynamic processes for the purposes of establishing the conditions of sustained high energy density operation and to project upper limits of power density. To extend operational time of electrode and contact surfaces.

6. Chemical Propulsion - To extend specific impulse and density, controllablity, and storage times.

PROSPECTIVE TECHNICAL APPROACHES:

1. Power Generation - Establish unified and comprehensive thermodynamic basis for comparing concepts. Characterize plasma production, radiation, conductivity, and instability mechanisms in the confines of compact space systems. Investigate chamber and window material degradation processes in terms of electrochemically enhanced aerothermochemistry mechanisms. Examine the material and fluid transport limits of aerodynamic windows. Investigate the basic physics limiting the application of multimegawatt chemical, beamed energy, etc sources to space operations. Establish models of explosively driven generators. Model the behavior of dielectrics at high temperature, as well as the coupling of the power sources to intermediate storage and conditioning systems. Develop models for the candidate nonconventional power sources capable to sustained space operations at the ten- to hundred-megawatt(electrical) level. Determine cross sections, dielectric strengths, film coefficients, surface modification processes, and annealing to support comprehensive modeling and model calculations.

2. Thermal Management - Explore potential of active cooling concepts. Establish a comprehensive mechanistic model of the droplet motion and radiation; explore concepts to eliminate electrostatic dispersion of

droplets. Analyze thermal isolation mechanisms taking advantage of advances in porosity and magnetic properties. Formulate heatpipe working fluids to operate over a wider range of temperatures. Establish transient models for pulse power systems.

3. Power Distribution and Energy Storage - Extend field theory models to enhance the pulse-coil power conversion and storage efficiency. Consider superconductivity mechanisms in terms of highest pulse-power requirements. Analyze novel power transmission and distribution concepts that take advantage of space station structure. Model transient couplings among power supply, storage, and distribution systems.

4. Beamed Energy - Model and characterize beamed energy absorption and combustion processes and concepts. Establish the basic mechanisms for processes such as circumferential radiation, absorptivity, and ignition. Conceptually analyze methods of magnetic plasma confinement and thermal protection of surfaces.

5. Electromagnetic Acceleration - Model plasma flow processes to establish the upper levels of power density. Categorize the interactions between plasma flow fields and surfaces in terms of comprehensive, multicomponent transport mechanisms and material loss mechanisms. Categorize conditions which interfere with communication bands and produce deposits on optical surfaces. Achieve low temperature, high velocity plasma production through deflagration acceleration.

6. Chemical Propulsion - Synthesize high energy-density fuels competitive with LH_2 but with less severe storage requirements. Extend the analytical models of reacting transonic flow to reduce nozzle length through radical contours. Establish the low pressure, short residence time limits of metallized fuels. Achieve continuous storage of deep cryogenic fuels using molecular absorption refrigeration. Evaluate combustion conditions leading to toxicity hazards. Establish the mechanisms for achieving the most efficient propulsive interactions from sequential detonations.

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* Abstract is not in this document

Omitted Intentionally per the Program manager

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